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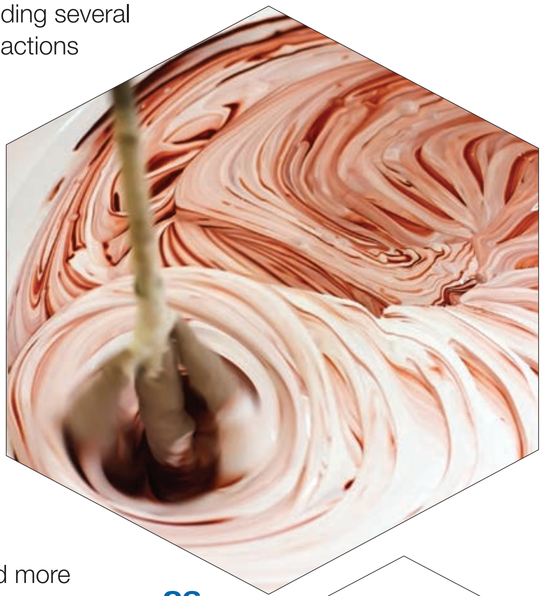
Cover Story

In the News

Technical and Practical



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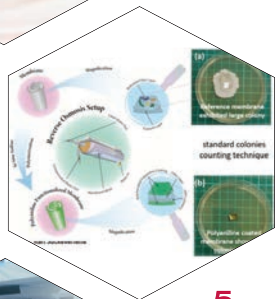

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Cover design: Tara Bekman

CHEMICAL ENGINEERING
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Editor's Page

'Green' chemistry winners

This year marks the 25th anniversary of the Green Chemistry Challenge Awards — a program that is sponsored by the U.S. Environmental Protection Agency's (EPA; www.epa.gov) Office of Chemical Safety and Pollution Prevention, and co-sponsored by the American Chemical Society (ACS; www.acs.org). The awards aim to recognize and promote achievements that reduce hazards to people and the environment, while also attaining economic benefits. The following five outstanding achievements have been named as the 2021 Green Chemistry Challenge Award winners.*

Greener Synthetic Pathways — **Merck & Co., Inc.** (www.merck.com) received this award for developing a more sustainable process for manufacturing gefapixant citrate, which is a medication for chronic cough. Merck was able to achieve a higher yield process with a six-fold reduction in raw material costs, while also replacing an alkylation step that involved hazardous materials. Merck implemented a measurement tool called process mass intensity (PMI) as a measure of process efficiency for biopharmaceutical production. The initial process had a PMI of 366, and the improved process registered a PMI of 88, an improvement by more than a factor of four.

Greener Reaction Condition — This award went to **Bristol Myers Squibb** (www.bms.com) for developing a new, sustainable class of chemical reagents for solid-phase synthesis that are derived from limonene, a waste product from discarded citrus peels. A key element in this technology is the use of phosphorus reagents instead of the traditional oxidation reaction. This change reduces the amount of reagent and solvent required and is said to improve the stability of the reagent and intermediate products. The need for specialized technology and shipping and storage has also been eliminated, since the phosphorus reagents are more tolerant to air and moisture.

Designing Greener Chemicals — **Colonial Chemical, Inc.** (www.colonialchemical.com) received this award for developing surfactant blends that are derived from plant-based materials, are biodegradable, and have shown the potential to replace ethylene oxide (EO) containing surfactants. The process uses only water as a solvent and consumes less energy than processes using petroleum-based raw materials. The surfactants are functionalized alkyl polyglucosides (APGs) that are said to provide cleaning performance that is equal to or better than alkylphenol ethoxylates (APEs), while avoiding the environmental issues associated with APEs.

Small Business — This award recognizes **XploSafe LLC** (www.xplosafe.com) for its novel sorbent that can capture ammonia, phosphate and nitrate from contaminated water. Various metal oxides, which can adsorb various nutrients, are combined and the material can be turned into granules and used as a time-release fertilizer. The technology offers cost and utility advantages over standard biological and chemical treatment solutions. Hydra Water Technologies, a spin-off from XploSafe, manufactures the material under the name PhosRox.

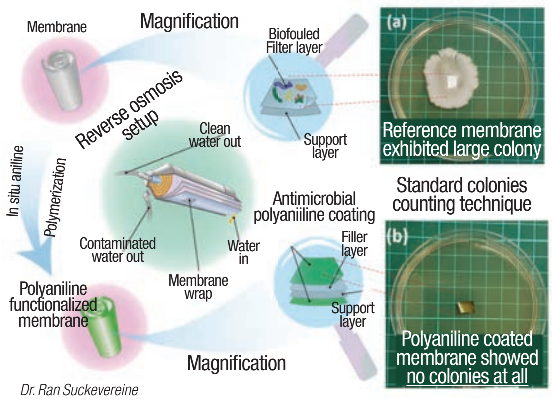
Academic — This honor was awarded to a team led by professor **Srikanth Pilla** of **Clemson University** (www.clemson.edu) for creating the first lignin-based non-isocyanate polyurethane foam. The lignin-based foam can be chemically recycled, and the catalyst can also be recycled. The innovative process to make this foam uses non-toxic, bio-based reagents, and does not use diisocyanates. ■

Dorothy Lozowski, Editorial Director

* Source: EPA; More details about the award process and the winners can be found on the EPA's website, www.epa.gov

Edited by:
Gerald Ondrey

Anti-biofouling coating for desalination membranes extends lifetimes



Dr. Ran Suckevereine

Buildup of biofouling on membranal surfaces necessitates treatments with corrosive chemicals, such as hydrochloric acid, and even replacement of membrane cartridges, which can be costly in desalination operations. A new coating, developed in the laboratory of Ran Suckevereine at Kinneret Academic College (Gallilee, Israel; www.kinneret.ac.il), is capable of preventing microbial growth on surfaces of commercially available desalination membranes, while maintaining the flowrate and salt rejection observed with the untreated membrane.

The use of coatings to prevent biofouling on membranes has been previously tried, but "coating materials can wash into the treated water if they are not strongly attached," explains Suckevereine. "Free-radical mechanisms can be used to attach active polymers to the membrane, but without special considerations, the free radicals may damage the membrane."

The group's approach overcomes a number of these issues. The coating is made from polyaniline that is polymerized in the presence of the membrane in such a way that it is chemically bound to the membrane. The Kinneret team used a unique polymerization technique, known as inverse emulsion polymerization, along with sonication, to allow the polymerization to proceed at faster rates, and to allow the polyaniline binding to occur without damaging the membrane.

Inverse emulsion polymerization involves a large organic phase containing the aniline monomer, and smaller aqueous phase containing free-radical initiators. Applying ultrasonic soundwaves with a sonicator creates tiny droplets of water within the organic phase, and the polymerization occurs at the water-solvent interphase.

With the small droplets, "there are lots of reaction sites, which increases the rate and yield of the polymerization," says Suckevereine. Also, the sonication creates free radicals, which allow the binding to the membrane. Since the membrane is present within the inverse emulsion, a thin (~80 nm) layer of polymer forms on the membrane surface.

In tests with *E. coli* bacteria and water from the Sea of Gallilee, Suckervereine's group found that the coating prevents microbial growth (photo), and allows the same flowrate and degree of salt rejection as untreated membrane. The team has scaled up the process beyond laboratory scale, but is currently working on another scaleup to a cubic-meter-sized reactor.

Recovering carbon black from waste tires

Until now, waste tires have been used mainly for recovering energy. Only small proportions of the carbon black contained in these tires are recycled, since the mineral ash generated by pyrolysis consists of about 20 wt.% of additives used to make the tires. A new process developed by the Fraunhofer Institute for Building Physics (IBP; Valley, Germany; www.ibp.fraunhofer.de) is able to isolate almost all of this ash, allowing both the carbon black and the minerals from the ash to be reused. The process was developed on behalf of RCB Nanotechnologies GmbH (Munich, Germany; www.recovered-carbon-black.com).

To purify the carbon-black/ash mixture created during the pyrolysis process, a wet chemical method is used. The (raw) carbon-black/ash mixture, together with various additives and a liquid, are blended in a reactor, and taken through a defined pressure and temperature curve. The parameters and additives are adjusted in such a way that only one particular mineral is selectively extracted from the mixture at a time. This demineralization process produces high-purity, recycled carbon black for use in tires and other rubber products, as well as colorants (masterbatch) for plastic applications, silicates, which can be used in the building materials industry or for dyes, for example, and also zinc salts for a broad range of applications.

A 200-L pilot plant will operate for the next two years at Fraunhofer IBP, aiming to make recovered carbon black usable for other industrial applications besides tires. The basic process has already been patented, and RCB Nanotechnologies GmbH is the exclusive licensee. The company is currently working on scaling up the process and the production hall is already built. The reactor volume for one production line is expected to be around 4,000 L, which will produce 400 kg/h of recycled carbon black from the ash, or 2,500 ton/yr. In the final expansion stage, the plant will have a capacity of 30,000 ton/yr.

TOXICOLOGY TESTING

The world's first toxicology-testing strategy without animal testing has been approved by the Organization for Economic Co-operation and Development (OECD; Paris, France; www.oecd.org). The testing strategy consists of three so-called alternative methods. They can be used to predict whether a substance causes allergic reactions in the skin. Unlike in the past, animal testing will no longer be necessary for this.

This testing strategy was developed and validated in a joint effort by BASF SE (Ludwigshafen, Germany; www.basf.com) and Givaudan (Vernier, Switzerland; www.givaudan.com). "For more than 10 years, we have been working towards this goal," says Robert Landsiedel, vice president, Special Toxicology, BASF. "We have taken a big step forward. Now we can also use alterna-

(Continues on p. 6)

tive methods to answer more complex toxicological questions without animal testing." Andreas Natsch, head of in vitro Molecular Screening at Givaudan adds: "This strategy has a better predictivity for human allergy risks as compared to traditional animal testing."

E-CRACKERS

A joint-technology program to electrically heat steam-cracker furnaces, which Dow, Inc. (Midland, Mich; www.dow.com) and Shell Chemicals (London, U.K.; www.shell.com) began in June 2020, is progressing forward. The joint program was awarded €3.5 million ($4.2 million) in MOOI (Mission-driven Research, Development and Innovation subsidy) scheme funding by the Netherlands Government. In addition, the partners have joined forces with The Netherlands Organization for Applied Scientific Research (TNO; The Hague; www.tno.nl) and the Institute for Sustainable Process Technology (ISPT; Amersfoort, both the Netherlands; https://ispt.eu). This multi-company collaboration aims to accelerate key milestones for the near-term progress and longer-term breakthroughs needed.

In the first year, the program has advanced electrification solutions for today's steam crackers while also pursuing game-changing technologies for novel designs of electrified crackers in the longer-term. Joint teams in the Netherlands and the U.S. have deployed their expertise in electrical design, metallurgy, hydrocarbon technology and computational fluid dynamics to narrow down concepts, validate emissions benefits, advance patents, demonstrate the durability of electric heating elements, and partner with equipment suppliers.

The companies are now evaluating construction of a multi-megawatt pilot plant, with potential startup in 2025, subject to investment support.

(Continues on p. 8)

Piloting a process that makes hydrogen and carbon from methane

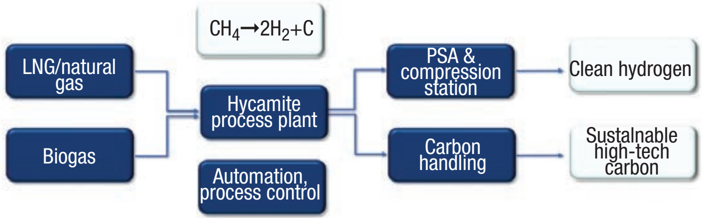
Next year, construction will begin on an industrial-scale pilot plant to further develop a new process that decomposes methane into H_2 and carbon. The process uses a thermo-catalytic decomposition (TCD) technology developed by Hycamite TCD Technologies Oy (Kokkola, Finland; www.hycamite.com). The pilot plant will be located in the Kokkola Industrial Park (KIP), which has the highest concentration of inorganic chemical industry in Northern Europe.

In the TCD process (diagram), natural gas or biogas is continuously fed to a fixed-bed or fluidized bed (or both) reactor operating at 500–800°C and 1 atm. In the reactor, CH_4 is split into H_2 and C using a proprietary catalyst that the company has developed over several years. H_2 is purified (>95%) by pressure-swing absorption (PSA), and the unreacted CH_4 is circulated back to the reactor. Solid carbon is discharged from the reactor, cooled and packaged. The technology can generate several different high-quality allotropes of carbon, and can be optimized for preferred allotropes.

Because the reactor is heated by hydrogen and renewable electricity, with heat recovery, there are zero CO_2 emissions generated in the process. According to CEO Laura Rahikka, TCD hydrogen technology has the highest H_2 yield per unit energy compared to steam methane reforming (SMR) and electrolysis of water. Based on the carbon product, the price of the H_2 generated is "highly competitive" compared to other technologies, says Rahikka.

"Our goal is to implement large-scale hydrogen production over the next couple of years, using our new technology," says Rahikka. "The hydrogen we generate can be used for clean energy production and for various industrial processes. Our output will enable companies to switch to hydrogen in the next few years, despite shortages in wind-powered hydrogen production that may continue for some time," she says.

Hycamite



This sustainable, supercharged catalyst cleans up mold

A family of oxidation catalysts known as TAML has been revamped to increase activity by several orders of magnitude, even at very dilute catalyst concentrations. Developed by Sudoc (Cambridge, Mass.; www.sudoc.com), these peroxidase-mimicking catalysts present a more environmentally sustainable option in challenging cleaning and treatment applications, such as mold treatment, where toxic chemicals are typically required, says Roger Berry, CEO of Sudoc. "Because of its oxidative characteristics, the catalyst acts as a 'super-cleaner.' Our team has formulated a very powerful mold cleaner that uses significantly less hypochlorite than other products on the market," adds Berry.

The key to TAML catalysts' performance alongside oxidants is an iron atom surrounded by a macrocyclic amide-containing ligand, which makes the catalyst extremely active in oxidation reactions, but also very resilient, especially compared to other transition-metal oxidation catalysts, explains Matt Mills, Sudoc's director of research and development. The combination of activity and resilience comes after decades of iterations to pinpoint the weak points in the macrocycle and formulate a structure optimized to survive in conditions where other catalysts would quickly burn up, but also where the homogeneous catalyst macrocycle can disappear from the environment once its job is complete. "Earlier versions of the catalyst had a closer ratio of catalyst activity to its self-destructiveness, so you could see the potential, but the latest versions greatly extend the ratio. So that decoupling was a major breakthrough," adds Berry.

Beyond resistance to oxidation and nucleophilic attack, the catalyst's structure is highly tunable, so it can be optimized for many environmental-remediation tasks. Sudoc is launching its first commercial product, a mold cleaner, later this year, and several demonstration projects are underway to test large-scale treatment. "There have been a wide variety of bench-scale studies looking at destroying pharmaceuticals, explosives, hormones and other substances. We're also treating wastewater with our technology and showing numerous different compounds that were present in the effluent that can get reduced, some almost to non-detectable levels," says Mills.

FOSSIL-FREE SPONGE IRON

A strategic partnership between Kanthal AB (Stockholm, Sweden; www.kanthal.com) and Hybrit aims to develop an electric gas-heating solution for the fossil-free hydrogen used to reduce iron ore in the Hybrit process. Hybrit (hydrogen breakthrough ironmaking technology) is a cooperation between the steel company SSAB, mining company LKAB and the energy company Vattenfall. Its aim is to replace the coal-based blast furnace process with a direct reduction process, based on H_2 produced with fossil-free electricity.

One of the challenges in the Hybrit process is the ability to preheat large amounts of H_2, and this is where Kanthal will contribute. "Many industries around the world are struggling to find a solution that can heat large amounts of gas right now," says says Anders Björklund, president, Kanthal. "With this collaboration, we can develop a viable solution together."

Currently, Hybrit operates a pilot plant in northern Sweden, and Kanthal is developing the first heater and preparing it for testing in the pilot plant. The heater will be in the 250-kW range. If it proves successful, it will be upgraded to a 1-MW version. The goal is to develop a large-scale heating solution that could heat high volumes of H_2 up to 1,000°C. The development project is supported by the Swedish Energy Agency.

In addition to the pilot plant, Hybrit plans for an industrial-scale demonstration plant, to be commissioned by 2026 and produce 1 million ton/yr of iron. If Kanthal's heating solution meets the technical, financial and time requirements of the pilot plant, it will be scaled up and installed in the demonstration plant.

MYCELIUM-BASED LEATHER

Leather and synthetic-leather production have a large negative environmental impact due to resource-intensive processes and hazardous chemicals used during production. One alternative is fungal mycelium, a bio-based raw material that can be sustainably processed into leather-like materials. Until now, however, increasing the production volume with current methods has been challenging due to mycelium cultivation taking place in a planar two-dimensional form that is limited in size.

Now, a team of researchers from VTT Technical Research Center of Finland Ltd (Espoo, Finland; www.vttresearch.com) has demonstrated that its technology enables the continuous manufacturing of mycelium leather sheets by the meter. The approach is applicable to industrial roll-to-roll production.

VTT's patent-pending technology for producing mycelium leather-alternative materials is based on growing mycelium in common bioreactors. The benefits of this approach are that liquid fermentation in bioreactors is easily scalable to commercial scales. VTT's film-making process enables continuous mycelium leather-alternative production using VTT's pilot equipment. The benefits of this

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A project to further develop solar-thermal-energy storage technology

Synhelion S.A. (Lugano, Switzerland; www.synhelion.com) and the Swiss Federal Laboratories for Materials Science and Technology (Empa; Dübendorf; www.empa.ch) are conducting a joint research project, co-funded by the Swiss Innovation Agency Innosuisse, to further develop a high-temperature energy-storage technology that is a key component in the production of climate-friendly solar fuels. The project will enable the cost-effective and scalable storage of high-temperature solar heat at over 1,000°C for the first time. The storage technology is expected to be used in Synhelion's first industrial-scale solar fuel production facility, which will be built in 2022.

Synhelion produces sustainable fuels, such as gasoline, diesel and kerosene that are compatible with conventional internal combustion engines and jet engines. The ETH Zurich spin-off has developed a solar thermochemical process based on process heat generated from concentrated sunlight to produce these synthetic fuels (see Solar Chemistry Heats Up, *Chem. Eng.*, March 2018, pp. 12–16). To enable the chemical reactors for solar fuel production to operate around the clock, a cost-effective, high-temperature thermal energy storage (TES) is needed. This solution stores part of the solar energy to be used during the night and cloudy periods, enabling continuous operation of the reactors, thereby significantly increasing plant capacity and drastically reducing capital expenditure.

Currently, there is no TES on the market that is compatible with the high temperatures, cycle times and heat-transfer fluid of Synhelion's technology. For this reason, Synhelion is further developing the solid heat-storage technology, enabling the storage of high-temperature solar heat of over 1,000°C in a cost-effective and scalable manner for the first time. As part of the research project with Empa, storage and insulation capabilities will be optimized in terms of material costs, high specific heat capacity and service life. Additionally, a design for Synhelion's industrial-scale solar-fuel plant is being developed.

Low-energy hydrogenation without H_2 gas

Hydrogenation is an important reaction in many sectors of the chemical process industries (CPI), but H_2 gas is not only expensive, its use requires considerable safety measures to prevent explosions. Significant cost savings could be achieved if hydrogenations did not require compressed H_2 gas. Researchers at the Dept. of Chemical Sciences, University of Johannesburg (South Africa; www.uj.ac.za) have taken a step in this direction by developing a safe, low-energy process for transforming nitrobenzene, a toxic waste product, into aniline, an important feedstock for many chemicals and medicines — without the need for compressed H_2.

The researchers use a so-called Pickering emulsion — an emulsion that is stabilized by solid particles — to convert nitrobenzene into aniline. As described in a recent issue of *Colloids and Surfaces*, the hydrogenation takes place at the aqueous-organic interface of the Pickering emulsion, where the solid catalyst particles also serve to stabilize the emulsion.

The catalyst consists of modified silica microspheres and palladium, as well as a bimetallic catalyst (PdM, where M = Co, Ni). The other two phases of the emulsion are toluene, which dissolves the nitrobenzene, and an aqueous solution of sodium borohydride. The stable droplets of the water-toluene emulsion act as microreactors for the reaction, with the $NaBH_4$ supplying the hydrogen needed for the reduction.

If the three phases are added together, but not mixed, the combination can be stored for days or weeks, says professor Reinout Meijboom. When the three phases are mixed into an emulsion, which takes a few seconds, the catalyst kick-starts the reaction. At the laboratory scale, the reaction takes about 2 h at room temperature.

The emulsion process has the potential to be a much safer industrial hydrogenation process than those currently in use, says Meijboom.

Collect more solar energy and waste heat for process water heating

A new technology developed by Enertopia Corp. (Kelowna, B.C., Canada; www.enertopia.com) aims to improve the efficiency of solar panels by collecting excess waste heat and using it to heat water. Besides improving energy output, the technology also significantly lengthens the useful lifespan of solar panels by reducing overheating.

Enertopia's technology involves outfitting the backside of a solar panel with a sponge-like heat-dissipative device made of ethylene propylene diene monomer (EPDM). "Basically, there's water flowing underneath the solar panels, which removes the excess heat, but in order to couple the panel to the EPDM rubber device and not shock the panel or break the glass, we have developed a breakthrough technology that actually acts like a one-way heat sink on the back of the panel," explains Mark Snyder, lead process technologies consultant for Enertopia. In some conditions, says Snyder, the EPDM device can take advantage of dewpoint differences and draw water out of the atmosphere, meaning that it can actually create water in addition to collecting waste heat. "If you have a large array, you could actually be making several thousands of gallons of water per day," he adds. On either side of an array of panels with the special EPDM medium applied, header lines gather water and pump it through a series of insulated tanks and solar-thermal booster panels made of the same EPDM medium, where the water can be heated as high as 220°F.

Enertopia is currently maturing the technology as part of an effort to create a closed-loop system for solar-powered direct lithium extraction (DLE) technologies, which are currently under review. The solar-absorption circuit provides carbon-neutral heating for process water, which is then used to remove lithium from impurities in a brine solution. The company is currently testing a demonstration system near Sacramento, Calif., that Snyder says has raised the efficiency of the solar panels by 20 to 25%. The company is also working on a 3-MW system to demonstrate the effectiveness of the system for agricultural use.

manufacturing method are consistent quality, competitive production price and reduced amounts of offcuts.

"The material has a leathery look and feel and can be as strong as animal leather. It also offers the possibility to be colored and patterned, and it does not contain any backing or supporting materials," says senior scientist Géza Szilvay.

The researchers are now working to improve tear strength and abrasion resistance by bio-based approaches. The first product applications for the material could be accessories, footwear and garments.

BONDING COMPOSITES

With the increasing demand for lightweight composite materials, the ability to bond together dissimilar materials, such as resins and metals is of growing importance. Although there are many methods available, such as

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bonding with liquid adhesives or hot-melt adhesives, or mechanical fastening with bolts, manufacturers have been demanding simpler bonding methods that maintain adhesive strength.

To meet these challenges, Showa Denko K.K. (SDK; Tokyo, Japan; www.sdk.co.jp) has developed WelQuick, a film-type adhesive component that eliminates the need for applying liquid components used for reactive adhesives. WelQuick is easy to handle, and shortens bonding time to a few seconds. Conventional adhesives require dozens of minutes, says the company.

WelQuick utilizes the phase change between solid and liquid, and materials can be joined by ultrasonic welding, electromagnetic induction welding and heat welding. It can bond resins (such as polycarbonate, polyethylene terephthalate and nylon) and metals (including aluminum, iron and copper). SDK has confirmed that WelQuick can achieve shear adhesive strength of more than 10 MPa with more than 40 combinations of base materials. ❐

Sustainable mining of raw materials from thermal springs

According to statistics from the World Bank, thousands of tons of valuable minerals are imported to Germany from Chile every year, including raw materials for lithium-ion batteries. But their extraction causes ecological and social problems. “The use of the limited freshwater resources in northern Chile for mining regularly fuels conflicts with the local population,” says professor Thomas Kohl from the Institute of Applied Geosciences (AGW) at the Karlsruhe Institute of Technology (KIT; Germany; www.kit.edu). “Northern Chile is one of the driest regions on earth, but has extensive geothermal resources," he says. "With a novel type of plant, it is not only possible to generate electricity in a climate-friendly way, but also to extract drinking water and even mineral resources at the same time.”

As part of BrineMine — a German-Chilean research project that began in 2019 with €1.5 million in funding from the Federal Ministry of Education and Research — the AGW team is developing the necessary strategies and technologies for extracting mineral resources, as well as drinking water, directly in geothermal power plants. One partner is the Fraunhofer Institute for Solar Energy Systems (ISE; Freiburg, Germany; www.ise.fraunhofer.de); which is developing the plant technology for later industrial use. In the process, heat from the geothermal brine is first used for energy recovery. The cooled liquid, which has a relatively low concentration, is then pre-concentrated by reverse osmosis, which also generates drinking water. The brine concentrate is then further concentrated by membrane distillation until it is saturated. “The thermal energy required for the entire process can be covered directly from the excess heat of the power plant process,” explains ISE project manager Joachim Koschikowski. A demonstration plant is now set up in a geothermal power plant in the Upper Rhine Graben and successfully integrates key components into ongoing power plant operations. The research is described in a recent issue of *Geothermics*. ■

Business News

Plant Watch

Chemours breaks ground on $93-million mining facility in Florida

July 14, 2021 — The Chemours Co. (Wilmington, Del.; www.chemours.com) recently held a groundbreaking ceremony for a new $93-million mining facility in Clay County, Fla. This site will give Chemours additional access to concentrated deposits of titanium and zircon mineral sands, which are used to produce titanium dioxide. Startup is anticipated by the fourth quarter of 2022.

Vynova to build potassium carbonate plant in Belgium

July 14, 2021 — Vynova Group (Tessenderlo, Belgium; www.vynova-group.com) will build a production plant for liquid potassium carbonate at its site in Tessenderlo, Belgium. The new plant, representing an investment of €4 million, is expected to be operational by mid-2022. Construction is due to start in the third quarter of 2021. The new facility will be the largest plant of its kind in Europe.

Shell starts up 10-MW green-hydrogen plant in Germany

July 13, 2021 — Royal Dutch Shell (The Hague, the Netherlands; www.shell.com) announced that its 10-MW water electrolysis plant has started operations at Shell Energy and Chemicals Park Rheinland in Wesseling, Germany. The plant will produce up to 1,300 metric tons per year (m.t./yr) of green hydrogen. Shell is also planning to build a 100-MW electrolysis plant at the site, with construction planned to start as soon as 2022.

Haldor Topsoe to build new catalyst plant in Texas

July 13, 2021 — Haldor Topsoe A/S (Lyngby, Denmark; www.topsoe.com) will build a new hydroprocessing-catalyst plant at the company's existing Bayport production site in Pasadena, Tex. The plant is designed to produce 15,000 m.t./yr of catalysts to meet increasing demand, both in traditional petroleum refining and the production of renewable diesel and jet fuel. The plant is expected to be fully operational in the first half of 2023.

Repsol to build two new polymers plants in Portugal

July 12, 2021 — Repsol S.A. (Madrid, Spain; www.repsol.com) will build two polymer materials plants at its Sines Industrial Complex in Portugal, representing an investment of €657 million. The facilities will be operational in 2025. The project includes a linear polyethylene plant and a polypropylene plant, each with a capacity of 300,000 m.t./yr.

Siemens to build one of Germany's largest green-hydrogen plants

July 12, 2021 — Siemens AG (Munich, Germany; www.siemens.com) has started construction on a hydrogen production plant with a capacity of 8.75 MW. The facility will produce up to 1,350 m.t./yr of hydrogen using only renewable energy. The new hydrogen plant is scheduled to go into operation in the summer of 2022.

MOL Group and Tatneft to construct new rubber bitumen plant in Tartarstan

July 12, 2021 — MOL Group (Budapest, Hungary; www.molgroup.info) and Tatneft (Almetyevsk, Republic of Tartarstan, Russia; www.tatneft.ru) have launched a joint project for a rubber bitumen plant in the Republic of Tatarstan, which will have a production capacity of about 20,000 m.t./yr. The companies have also agreed to establish a joint venture that, besides manufacturing and selling rubber bitumen, will also pursue technology licensing.

Dow to increase propylene glycol production capacity in Thailand

July 6, 2021 — Dow, Inc. (Midland, Mich.; www.dow.com) announced that its Polyurethanes & Construction Chemicals business plans to increase propylene glycol (PG) capacity at its existing facility in Map Ta Phut, Thailand by 80,000 m.t./yr, bringing total capacity to 250,000 m.t./yr. Once complete, this expansion will make the Dow Map Ta Phut PG facility the largest of its kind in the Asia Pacific region. The capacity expansion is expected to come online in 2024.

Kemira to increase production of water-treatment chemicals in China

July 1, 2021 —Kemira Oyj (Helsinki, Finland; www.kemira.com) is increasing production capacity of water-treatment chemicals in Yanzhou, China. Kemira has started to build a new sodium-hypochlorite production unit at Yanzhou site. It is expected to start commercial production in January 2022. Kemira is also finalizing the pre-engineering phase for an investment to increase the production of polyaluminum chloride (PAC) at Yanzhou.

Röhm to build MMA plant on U.S Gulf Coast

June 30, 2021 — Röhm GmbH (Darmstadt, Germany; www.roehm.com) has started engineering and construction work on a new production plant for methyl methacrylate (MMA) in Bay City, Tex. Röhm expects mechanical completion in 2023. The new plant will have a production capacity of 250,000 m.t./yr.

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Air Liquide to build €70-million gases plant in Wuhan

June 28, 2021 — Air Liquide S.A. (Paris; www.airliquide.com) will invest around €70 million to build a new gases plant in Wuhan, China to supply a major microchip maker. Air Liquide will build, own and operate this ultra-high-purity industrial-gas plant, which will produce 52,000 m^3/h of nitrogen, as well as oxygen and argon, among other ultra-high purity gases. The plant is planned to be operational in 2022.

Indorama adds PNDA production unit in Alabama

June 21, 2021 — Indorama Ventures Xylenes & PTA, LLC (IVXP), a subsidiary of Indorama Ventures Ltd. (Bangkok, Thailand; www.indoramaventures.com), announced a new production unit for purified 2,6-naphthalene dicarboxylic acid (PNDA), which will make IVXP the world's largest PNDA producer. The unit is located at IVXP's integrated manufacturing site in Decatur, Ala.

Mergers & Acquisitions

Sasol sells its sodium cyanide business

July 12, 2021 — Sasol Ltd. (Johannesburg, South Africa; www.sasol.com) has concluded an agreement to sell its sodium cyanide business to a South African subsidiary of Draslovka Holding a.s., a Czech-based company specializing in cyanide production for R1.46 billion (around $101 million). The transaction is expected to close in the first half of 2022.

Enterprise acquires ethylene business from NOVA Chemicals

July 6, 2021 — Enterprise Products Partners L.P. (Houston; www.enterpriseproducts.com) and NOVA Chemicals Corp. (Calgary, Alta., Canada; www.novachem.com) announced that a subsidiary of Enterprise has acquired a wholly owned subsidiary of NOVA Chemicals that operates an ethylene storage business and trading hub in Mont Belvieu, Tex. This acquisition gives Enterprise ownership of the largest ethylene market hub in Texas.

BASF acquires catalyst-recycling plant in Texas

July 6, 2021 — BASF SE (Ludwigshafen, Germany; www.basf.com) has expanded its chemical catalyst recycling capacity and capability with the acquisition of Zodiac Enterprises LLC, located in Caldwell, Tex. Zodiac's site recycles precious metals from industrial scrap, primarily chemical catalysts, and will complement BASF's existing precious-metal recycling operations in Seneca, South Carolina.

Air Liquide acquires world's largest oxygen-production site

June 25, 2021 — Air Liquide has finalized the acquisition from Sasol of 16 air separation units (ASUs) located in Secunda, South Africa. Air Liquide will operate this site — the biggest oxygen production site in the world — with a plan to reduce its CO_2 emissions by 30 to 40% within the next ten years. The initial investment is approximately €480 million. The 16 ASUs have a total installed capacity of 42,000 m.t./d. ■

Mary Page Bailey

Electric Vehicles Drive Performance Polymers

Higher-volume production of battery-powered vehicles is driving the development of high-performance polymers with improved properties to meet the needs of electric propulsion

The market for battery-powered electric vehicles (BEVs) has grown rapidly over the past five years. According to a recent analysis by market research firm IDtechEX (Cambridge, U.K.; www.idtechex.com), global sales of BEVs in 2020 were 5.5 times larger than in 2015, and BEV sales remained strong in 2020, despite the pandemic. As sales continue to increase, BEV technology is advancing in parallel, with battery capacity and energy density growing while vehicles become more connected and more autonomous.

Expansion of electric vehicles and vehicle-battery manufacturing has driven higher demand for high-performance polymers and polymer composites that exhibit specific properties required for safe and effective operation. The American Chemistry Council (ACC; Washington, D.C.; www.americanchemistry.com) states that hybridization and electrification will increase demands for efficiency, battery longevity, weight and space savings, as well as safety enhancements. Among the key properties for plastics used in BEV applications are high dielectric strength, high strength-to-weight ratio, flame retardance, impact resistance and others. Chemical manufacturers are continuing to develop new polymer grades, new additives and processing methods to meet the requirements of electric vehicles.

E-mobility requirements

Electromobility (e-mobility; referring to the use of technologies that allow electric propulsion of vehicles) has introduced new demands on the polymers used to make vehicle components. "There is a new set of requirements for materials in e-mobility," says Brian Vargo, BASF E&E & eMobility segment manager at BASF Performance Materials (Wyandotte, Mich.; www.basf.com), "including electrical conductance, electromagnetic interference [EMI] shielding, flame retardance, dielectric strength (ability of insulating materials to withstand high electric fields without losing insulating properties) and others, and this creates opportunities for plastics to be introduced into EVs [electric vehicles]."

Dirk Heinrich, vice president of automotive and e-mobility at Evonik High Performance Polymers GmbH (Darmstadt, Germany; www.evonik.com) agrees that EVs have been a big driver for performance plastics because of their unique needs, including handling new types of fluids, improved electric isolation, specific coloring and more. "There are many small and sometimes subtle differences between EVs and conventional automobiles that lead to more plastics being required for EVs. One small example of this is that the fluid cooling lines for BEVs need to have larger diameters and wall thicknesses, as well as be longer, than those in conventional engines." The sum of many similar examples at higher sales volumes leads to marked increases in plastics demand.

Darpan Parikh, a global product management leader in SABIC's (Al-Jubail, Saudi Arabia; www.sabic.com) specialties business, summarizes by saying "EV batteries bring additional safety requirements for chassis and structural members, and the need for lightweighting for long-range drive capability without compromising on crash performance."

At the same time, both BEVs and internal combustion engine (ICE) automobiles are adding a range of driver-assistance technologies, such as lane-centering, automatic braking and autonomous driving, that require specialized sensors, connectors and camera, adding new potential applications for performance polymers. Further, compounds and materials that address issues of noise, vibration and harshness (NVH) in the cars' interior are important.

A significant and ongoing transition that has been occurring in recent years is the shift to designing EVs from scratch, rather than trying to introduce electric-propulsion components into vehicles that were originally designed as ICE vehicles, explains Chris Korson, chassis and structural market segment manager at BASF Performance Materials. "The initial generations of commercial EVs were just trying to put batteries into the existing vehicle bodies. Newer EVs have changing architectures that are designed to be battery-powered from the beginning."

This design flexibility has led to new opportunities for polymer composites, including glass-reinforced polyurethanes as lighter weight replacements for metal parts. "Electric vehicle designs actually use more straight parts in their architecture," says BASF's Vargo, "which lend themselves to the use of polymer composites, such as glass-reinforced polyurethanes."

The fundamental shift from propulsion by fuel combustion to propulsion by battery has also placed an emphasis on balancing cost and performance, and has highlighted the importance of plastic materials (Figure 1). Dhanendra Nagwanshi, global automotive leader, EV Bat-

FiGURE 1. The shift from propulsion by liquid fuels to propulsion by battery has highlighted the importance of plastic materials with specific properties

teries & Electrical segment, SABIC's Petrochemicals business explains: "The battery pack is the most expensive assembly ever fitted to a vehicle. At the same time, mass [of the car] is an important variable — more mass means more energy required. All of a sudden, you need more battery storage, bigger brakes and so on."

"Despite the industry's best efforts," Nagwanshi says, "the addition of new technology and content continues to increase the overall curb weight of vehicles. The good thing about thermoplastic materials is their powerful combination of structural strength and low density. When you can remove mass and weight by, for example, replacing aluminum in battery packs with plastic, you can theoretically reach a point where battery cells can be removed because you no longer need as much energy for the same amount of range."

In addition, Nagwanshi points out, thermoplastics can contribute to additional cost savings by eliminating the need for adhesives and fasteners, and for die casting, welding and other processes.

Generally, the polymer types that are used for automotive applications have been known for quite awhile, says Bert Havenith, market intelligence and sustainability director at DSM N.V. (Geleen, the Netherlands; www.dsm.com). "But there has been significant innovation in ways to functionalize the materials through compounding processes so that they are able to exhibit improved properties for a wide variety of parameters. DSM, among others, has been working on improving specific properties so the polymers can be used in new applications," Havenith explains.

In an example of the increased demand for compounding of engineered plastics, Celanese Corp. (Irving, Tex.; www.celanese.com), announced a three-year plan to expand engineered materials compounding capacities at the company's Asia facilities, including the locations of Nanjing, China; Suzhou, China; and Silvassa, India. The initiative will add approximately 52,000 tons of compounding and long-fiber thermoplastics (LFT) capacity at the company's Nanjing chemical complex by the second half of 2023, as well as nylon compounding capacity at the Suzhou facility in 2022.

Glass-reinforced plastics

For making metal-replacement structural components in BEVs, where strength and stiffness at light weights is a premium, glass fibers are among the most common materials found in plastics. Significant focus has been leveled at processing glass-reinforced plastics, with the automobile market a major emphasis. BASF's Korson points out the impact of one kind of processing technique, known as pultrusion, on EVs. "New EV architectures lend themselves to pultrusion-made parts," he says, "and BASF has done a lot of work on pultrusion processing for composite materials, and have pushed pultrusion to achieve higher throughputs."

Pultrusion is a processing technique in which glass fibers are pulled through a bath of polymer resin.

Earlier this year, BASF introduced serial production of glass-fiber polyurethane parts made in a pultrusion process. "There are lots of opportunities in the future for pultrusion materials in EVs," Korson says. Another important factor in the adoption of pultrusion in the automotive market is the ability to model pultruded components in computer simulation to accurately predict the behavior in the full vehicle system. This is important for original equipment manufacturers (OEMs) and Tier 1 suppliers to design pultruded parts early in the vehicle development. Engineers are also working on ways to modify the glass fibers before they are introduced into the resin bath for different properties based on the applications needs.

Evonik recently introduced a number of products that will be used in the BEV market, including a new polyamide-12 polymer of the group's Vestamid L grades, a glass-reinforced, electrically conductive PA12 molding compound that was developed in particular for the injection molding of connecting elements for fuel line systems (such as quick connectors). The electrical conductivity of the new Vestamid L changes only slightly on contact with fuels, even if they contain alcohol. This is of great importance for use in fuel-conducting systems, Evonik says.

Lightweighting

Automotive engineers have long known the relationship between lowering vehicle weight and raising fuel economy. A rule of thumb in the auto industry has been that for a 10% reduction in weight, the fuel efficiency of the vehicle improves by 6–8%. In BEVs, vehicle lightweighting allows longer ranges for a given battery size or achieving the same range with a smaller (and therefore less costly) battery.

"Lightweighting by replacing metal parts with plastics is a priority across the board for vehicles, but most of the 'low-hanging fruit' in this area has been realized already," says Mark Jablonka, application technology leader for transportation at Dow Packaging and Specialty Plastics (Lake Jackson, Tex.; www.dow.com). Among the implications for this is that BEV makers are looking at every existing component for ways to cut weight. "The use of TPO [thermoplastic olefin; polypropylene (PP)-based composites containing

PP, elastomers and reinforcements] in automobiles has expanded greatly over the past 25 years, but further expansion into new applications, including those in BEVs, has required more innovation," Jablonka remarks.

Of the 25 products in Dow's Engage portfolio of TPO impact modifiers, Engage 11000 is the newest. Dow recently introduced the 11000 series of its Engage polymer product portfolio as a way to expand the usage space for PP and TPO in automotive applications. Engage is an ethylene-octene copolymer produced using Dow's single-site catalyst technology that is blended with PP and reinforcement materials. The concept behind the Engage 11000 series development was to arrange the co-monomers on the polymer chain in a specialized way to decrease the glass-transition temperature of the polymer, Jablonka explains. "The objective is to move the glass transition temperature lower to improve low temperature toughness while moving the melting temperature outside the normal operating range of the material to reduce thermal expansion," he says.

PP has a relatively large coefficient of linear thermal expansion (CLTE), so to be used for automotive parts with acceptable design appeal, such as body panels, it needs to be modified to minimize CLTE so that the small gaps between the panels, can be small, for example. Lower CLTE also avoids fatigue issues and cracking when TPOs are welded to other lower CLTE materials.

Another advantage of the Engage 11000 series is the superior melt flow properties it enables during processing due to its high impact efficiency, Jablonka says, which allows more complex geometries in the components to be made from it. The material has been launched commercially and is currently being incorporated into BEV and ICE vehicles. "Expanding the usage space of TPOs for lightweighting means there will be continued demand growth for plastics in vehicles," Jablonka says.

According to Dow's Jablonka, among the goals is more efficient impact modifiers with resins that flow well for processing, and have low-temperature toughness without embrittlement. Other plastics have potentially poor melt flow, but TPO can be used for more applications. "There's going to be continued growth in plastics due to lightweighting expanding usage space of the PP and TPO," Jablonka says.

Safety and flame retardance

The growing electrification of vehicles has made vehicle safety a particular concern, especially with the potential for battery fires and thermal runaway, many experts agree (Figure 2). "Vehicle safety can be particularly important when you look at the need to protect the battery system during a crash, including side impacts," SABIC's Parikh says.

"The possibility of battery fires

FIGURE 2. The possibility of battery fires has made flame retardance a critical property for vehicle safety in EVs

has pushed plastics makers to view flame retardance as a critical feature for EV components," says Sandra Reemers, vice president of R&D at Evonik High Performance Polymers.

BASF's Korson adds, "Many of the applications for performance plastics appear in the batteries, where thermal runaway protection is key."

Thermal management of the battery and improved flame-retardant properties are partly related to higher voltages observed in EVs. Bert Havenith, from DSM, says, the voltages experienced in modern electric vehicles are orders of magnitude higher than those seen in conventional vehicles, so there is a huge need for improved electrical properties, such as higher dielectric strength, higher comparative tracking index (CTI), a measure of the amount of voltage an insulator can withstand with 50 drops of water without tracking (electrical breakdown) values, as well as better flame-retardant properties.

SABIC's Nagwanshi says "We have developed and tailored specific resins from our polymer portfolio that we have modeled using computer-aided engineering (CAE) tools to ensure they comply with safety requirements and regulations, whether these apply to a crash scenario or some sort of system failure leading to a fire in the battery pack."

China's new GB 38031-2020 standard requires a battery cell that has caught fire to delay propagating to other cells or battery modules for up to five minutes so occupants have time to exit the vehicle, Nagwanshi says, and "SABIC's polymer materials can be key in meeting this requirement and upcoming safety regulations in other countries."

SABIC has also developed a process for adding flame retardancy to resins. "The process features exceptional dispersion of the additive within the resin," says SABIC's Nagwanshi, "and that ensures uniform flame-retardant protection across the entire part."

An example of this resin technology for EV battery pack applications is SABIC's introduction of non-halogenated flame retardant Stamax resins for various electrification components. Because of its unique character, Stamax FR resin delivers a higher level of fire shielding protection, SABIC says. The exceptional dispersion and distribution of the FR additive within the polymer matrix, even at high loadings, helps maintain structural integrity of EV battery components. "This is not possible with competitive technologies, which would require halogenated FR chemistry to produce the same results," Nagwanshi says.

Temperature resistance is also a key property for new grades of SABIC's Noryl GTX resin family. SABIC's Parikh says, "The expanded temperature range of Notyl GTX resin has the potential to provide value to the OEMs at both ends of the temperature spectrum. The high-temperature resistance of the material allows for plastic components to be assembled to the frame of a vehicle prior to eCoat or along with the body of a vehicle for on-line painting. The low-temperature ductile performance of the material enables more predictable and repeatable energy absorption at low-temperature impacts. This predictability can help engineers optimize their designs and contribute to improved vehicle and occupant safety."

SABIC's Parikh continues, "In addition to temperature and impact resistance, our non-halogenated Noryl resins offers flame retardancy for battery covers, modules, electrical enclosure and other EV battery components. Noryl GTX resin can also be used for energy absorbers to aid in crash protection."

Flame retardancy in plastics also has implications for rapid charging, which is a key aspect of successful electromobility. New standards allow for charging up to 350 kW, which reduces charging time to minutes, but it also requires different materials for the equipment. In these applications, Evonik's flame-resistant Vestamid PA12 and Vestakeep polyether ether ketone (PEEK) are suitable for use as insulation for cables or busbars in the battery module or electric motor, and as plug components for high-voltage charging.

Sustainability

"The transition toward a circular economy for industrial goods will require the automotive industry and its suppliers to rethink the ways that vehicles and their materials are designed, constructed, used, and handled at end of life," says ACC.

Dow's Mark Jablonka agrees that the final big topic is circularity. "How do you make sure, at end of life, that your materials are not ending up in landfill?" he says. Designing for circularity is a tough challenge for the industry overall, and a priority for Dow. "We want to make sure all of the materials on the vehicle end up being recycled, either mechanically, or by using advanced recycling techniques like pyrolysis and gasification with the lowest carbon footprint."

DSM has also focused heavily on sustainability, including reducing carbon footprints of products and deriving monomers from recycled waste or from bio-sources. DSM has pledged to offer bio-based or recycled versions of all of its products by 2030. ■

Scott Jenkins

Editor's note: Additional comments regarding polymer use in EVs can be found in an extended version of this article at www.chemengonline.com.

Digitalization of Heat Transfer Fluid Systems

Department Editor: Scott Jenkins

The spread of COVID-19 opened the world's eyes to the weakness of much of its infrastructure and drove home the important role operators and engineers play in keeping manufacturing plants running. These unsung heroes were challenged with the difficult logistics of meeting production schedules and maintenance requirements while mitigating the spread of the coronavirus.

The pandemic also highlighted the need for digitally connected plants and operations. By digitally enhancing heat transfer fluid (HTF) systems, operation managers and engineers can be equipped with richer data to manage their production and maintenance more effectively and safely. In this way, they can monitor and forecast fluid testing issues related to acid number, moisture, viscosity and other parameters — all of which can impact production schedules and maintenance operations.

Despite the challenges of COVID-19, strict quarantine practices and modified work schedules allowed plants to continue normal operation by having essential workers on-site. But plants would have benefited from technology platforms that enabled productivity from afar. Not only are digitally enabled tools more convenient to monitor and track systems, they also give plant managers the ability to look across systems at various locations, fluids and applications to gain more insights. They enable managers to answer key questions like: "Are we operating most efficiently?" and "Are we maximizing the life of our fluid?"

The functions listed below are among the expectations plant managers and engineers struggled with when monitoring and tracking heat transfer systems during the unconventional operating conditions of the pandemic.

Production schedules. Digital tools that gather data and compile a dashboard of metrics and alerts for any subsystem within the plant help ensure production schedules are met, even when daily routines are disrupted.

Maintenance schedules. Ensuring efficient maintenance and having a view of future performance trends is also critical to productivity. Organized knowledge of past actions and results is important to understand how to resolve future challenges more efficiently.

Plant and system efficiency. Regardless of markets and global conditions, driving efficiency is critical to remaining competitive. Digital tools can allow operators to easily understand systems' conditions at a glance.

Training. Teams have experienced various shifts in roles and responsibilities to maintain operations. For this reason, there is a need for in-depth training materials to quickly bring your team up to speed.

Safety. Safety in manufacturing is critical to ensure an engaged workforce but also allows for the best overall productivity. Insights that proactively highlight potential safety challenges are invaluable.

HTF maintenance

When it comes to digitally connected HTF systems, the lessons learned from operating during the pandemic can be applied as normal operations resume to further improve day-to-day operations. Furthermore, all critical decisions involving heat transfer fluids have daily consequences for operators and engineers. The items listed below are some key best practices and recommendations to help ensure optimal performance of your HTF systems.

Improvements to digital monitoring capabilities. Production operations are likely already digitally enabled with programmable logic controllers (PLCs), distributed control systems (DCSs) and so on. To remain competitive, all companies should continue to explore and deploy more advanced digital tools to drive continued efficiency when it comes to monitoring viscosity, acid numbers, moisture content, flash point and more.

Annual fluid testing. Performing yearly fluid analysis offers a baseline for your system's performance. Digitally prompted or scheduled reminders facilitate compliance.

Actionable recommendations. Test results are valuable, but recommendations based on the results from experienced partners are even more valuable. Artificial intelligence and machine learning supported by vendor partners can help facilities receive the best recommendations for optimal fluid performance. For example, by analyzing moisture content trends, facilities can identify potential issues, such as heat exchanger pinhole leaks, that could result in an unplanned shutdown.

Easy-to-read sample analysis reports. Adopting a digitally enabled platform that provides easier-to-read sample analysis reports allows users to quickly scan key system performance metrics and know if action is required.

Sample analysis historical data. Data and digital trends can help quickly identify systematic or recurring issues based on current system performance compared to past performance. This includes trend recognition of viscosity and moisture content, inconsistent temperature or accelerated degradation.

Maintenance tracking and troubleshooting. Along with historical data, access to past maintenance activities allows engineers and operators to repeat actions, correct issues, or spot new issues. Also, tagging maintenance activities with the personnel who took action provides new employees with a network to discuss current activities. Preventive maintenance systems can begin to do this, but inclusive digital HTF maintenance systems that couple data and maintenance history with actionable recommendations are also available. ■

Editor's note: Content authored by Kapil Bathla, technical service and application development representative, Eastman Heat Transfer Fluids..

Production of Nitrogen from Air

By Intratec Solutions

Nitrogen (N_2) makes up 78% of ambient air (20.95% of air is oxygen). N_2 is an inert (non-flammable) gas used in industrial plants to prevent undesirable chemical reactions from occurring. Nitrogen is the most common inert gas used in the chemical process industries, due to its high natural abundance and low relative cost.

Major uses of N_2 include several in metallurgy: for heat treatments; as an alloy constituent; for scavenging; and as a protective gas; as well as in heat treatment. N_2 is also used as an inert gas in shielding and firefighting, in food storage and in processing. Nitrogen can be used in the manufacture of other products, including ammonia.

Most N_2 is produced onsite at industrial facilities, for local consumption. However, it may be stored and transported as a gas or a liquid, at cryogenic temperatures. High-pressure cylinders or cylinder clusters can be used for storage and shipping of small quantities of nitrogen gas. Liquid nitrogen can be transported and shipped in specially insulated storage vessels (small quantities) or by road and rail tankers (large quantities).

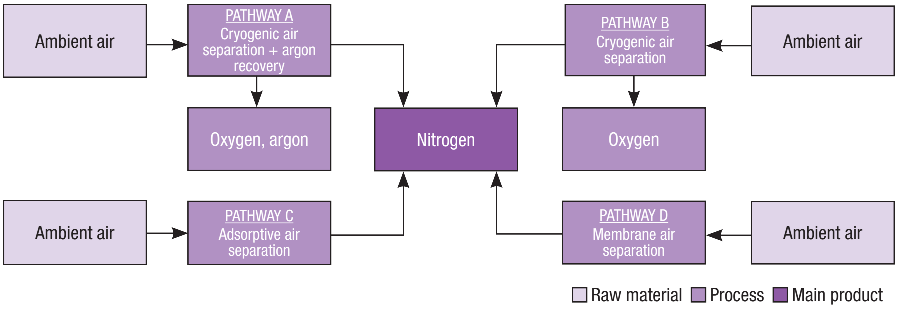


FIGURE 2. Cryogenic separation is used to produce gases from air, but other routes exist

Production process

The process of recovering N_2 from air comprises three major sections: (1) purification; (2) refrigeration; and (3) rectification (Figure 1) .

Purification. Initially, the air is purified from dust particles, carbon dioxide and water. This is accomplished by compressing the air, passing it through a heat exchanger (causing water condensation) and then through an adsorbent bed of molecular sieve for the removal of water, carbon dioxide and traces of other impurities.

Refrigeration. At this point, the purified air is cooled down/liquefied, as required for rectification steps downstream. This step is conducted in a plate-fin heat exchanger, using refrigeration values contained in the products (oxygen, nitrogen) and waste (nitrogen) streams.

Rectification. The last step in the process consists in submitting the cooled/liquified air to a fractional distillation carried out in two columns for nitrogen-oxygen separation, operating at different pressures, in such a way that nitrogen is distilled as a vapor and oxygen is obtained as a liquid. In addition, while oxygen and argon have close boiling points, a third column is used exclusively for the removal of that contaminant, vented to the atmosphere.

The main product obtained in the process under analysis here is gaseous, high-purity N_2 (the product gas is greater than 99.7% N_2), at 60 bars absolute.

Production pathways

Millions of tons of N_2 are isolated from atmospheric air every year, through different separation processes that are selected according to the production scale and purity required (Figure 2). The production of large quantities of relatively pure nitrogen is carried out, mostly, through cryogenic distillation. On the other hand, moderate volumes of low-purity nitrogen are commonly produced via pressure-swing adsorption and membrane permeation.

In addition to nitrogen, oxygen (O_2) and argon (Ar) can also be generated commercially in air-separation processes using cryogenic distillation and argon recovery units. Oxygen is also produced by vacuum-swing adsorption (VSA). ■

Edited by Scott Jenkins

Editor's note: Content for this column was originally developed by Intratec Solutions LLC (Houston; www.intratec.us) and is edited by *Chemical Engineering*. The analyses presented are based on publicly available and non-confidential information. The content represents the opinions of Intratec only. More information about the methodology for preparing the analyses can be found, along with terms of use, at www.intratec.us/che.

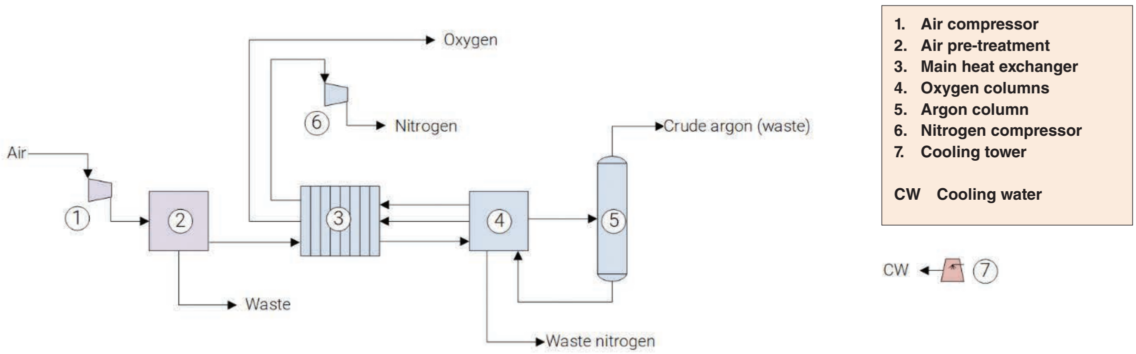
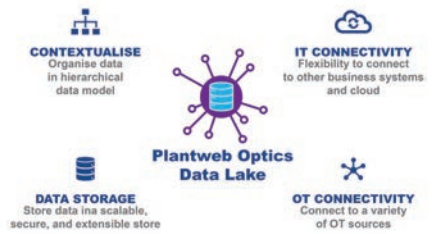


FIGURE 2. The diagram shows the process for producing nitrogen from ambient air

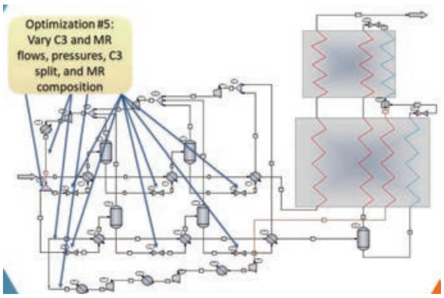
Focus on Software



Emerson Automation Solutions

Enterprise-level software simplifies data management

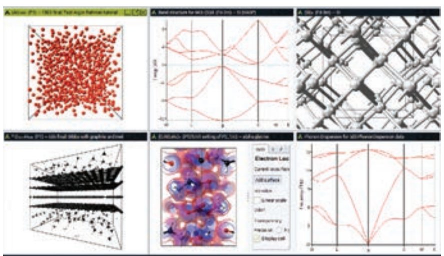
Last month, this company launched its Plantweb Optics Data Lake (photo), an enterprise-level data-management software solution that helps manufacturers reduce data complexity so that they can fully leverage operations data across a production site or from multiple sites to improve profitability enterprise-wide. This new advanced data-management solution securely identifies, collects and contextualizes disparate data, at scale, either on-premises or using cloud technology. Today, this valuable manufacturing data is often in different formats and siloed across a plant, posing significant impediments to a company's digital transformation initiatives. By effectively unifying this data, companies can establish a sound data foundation that can be leveraged by various digital solutions. — *Emerson Automation Solutions, Austin, Tex.*
www.emerson.com



Chemstations

Run simulations faster with this software

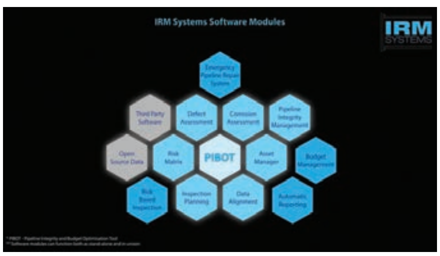
Computing power has increased significantly since the early days of process simulation. However, CPU clock speed is not the driving factor anymore; it is number of cores. The ability to parallelize calculations to all the available CPU cores, as CHEMCAD NXT (photo) can, is the key to running orders of magnitude faster than before. Using CHEMCAD NXT's Simultaneous Modular SQP Optimizer (which includes mixed-integer variables), companies can build optimizations directly into simulations they are already using for their work. Most chemical engineers are familiar with flowsheeting in a simulator, and most also understand the principles of optimization. Engineers also need confidence that the optimum found by the model is the global optimum. CHEMCAD NXT handles this by parallelizing a large number of starting positions. Multiple restarts are performed until several solutions converge within set tolerances. Therefore, CHEMCAD NXT's calculation speed increases the odds of finding the global optimum in a reasonable amount of time and each simulation run is extremely fast. The improvement in run-time for a complex optimization is on the order of 7–10 times faster from single-threaded to six-core calculation. Machines with more cores will give relatively similar performance increases, depending on simulation complexity. — *Chemstations, Inc., Houston*
www.chemstations.com



Materials Design

New software includes ML for designing materials

Last month, this company released MedeA 3.3 — Material Intelligence (photo). With the integrated and intuitive MedeA Environment, researchers build quantum-mechanical descriptions of systems using VASP 6, create machine-learning (ML) based potentials to capture the resulting energy surface, employ these descriptions in large length and time scale simulations using the LAMMPS package, and analyze results interactively. MedeA 3.3 includes updates to key server codes including: VASP 6.2.1, LAMMPS-29Oct20, and GIBBS 9.7.4, increased platform support, and a range of performance enhancements and productivity features throughout. Additional enhancements facilitate the evaluation of vibrational entropy contributions to system free energy, model construction and editing improvements, and enhanced and extended parameter sets for atomistic organic (PCFF+) and mesoscopic systems. — *Materials Design, Inc., San Diego, Calif.*
www.materialsdesign.com



Independent Risk Management Systems

New pipeline integrity and budget-optimization tool

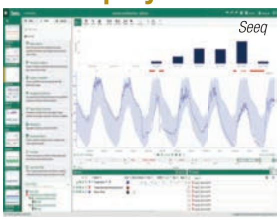
The Pipeline Integrity & Budget Optimization Tool (PIBOT; photo) is a new modular software package that reduces time and cost associated with carrying out a diverse range of pipeline-integrity, engineering and management activities via data management, integration and smart data analytics. This software solution makes it possible to instantly clean, structure, align, standardize and visualize data, in addition to carrying out pipeline integrity management and smart data analyt-

ics, says the company. For example, you could automate the process from inputting data to assessing risk, determining inspection intervals, and producing reports, all in a traceable, transparent way. As a result, operators benefit by working from enhanced data analysis that provides more accurate degradation forecasting and comprehensive risk assessments. — *Independent Risk Management Systems B.V., Delft, the Netherlands*
www.irm-sys.com

A new platform for advanced control and estimation

Platform for Advanced Control and Estimation R5.03 (photo) is an OpreX Asset Operations and Optimization solution that improves plant systems interoperability and security through support of the Open Platform Communications Unified Architecture (OPC UA) communication standard. Released in June, the platform was developed by this company and Shell. It is a software suite that brings together Shell's advanced plant process control technology and this company's real-time control technology to help users improve productivity by increasing product yield and reducing energy consumption. This version upgrade supports OPC UA, the latest version of a communication standard that improves plant systems interoperability and security, and provides the basis for digital transformation to help customers transition to industrial autonomy. OPC UA is recognized as a communication standard for Industry 4.0, benefitting from high security and scalability without hardware or OS dependence. The new version also includes a new BLC model that employs proportional integral differential (PID) control logic. — *Yokogawa Electric Corp., Tokyo, Japan*
www.yokogawa.com

From individual plants to cloud deployments



In March, this company introduced a new packaging of Seeq features and applications as Seeq Team and Seeq Enterprise editions (photo). These editions address the needs of users from a local water utility to a multi-national chemical, pharmaceutical or oil-and-gas company. Both Seeq editions, which run best as software as service (SaaS) on Amazon Web Service (AWS) or Microsoft Azure, represent the culmination of learning and experiences with hundreds of Seeq deployments in process manufacturing organizations. For these manufacturers, Seeq enables advanced analytics insights to improve production and business outcomes across their organizations. Seeq Cortex, a renaming of Seeq Server, is included in both editions and is the execution engine that delivers key features, including multi-source and type data connectivity, security, calculation scalability and other features. Seeq Cortex ensures immediate and long-term support for user data architectures and IT requirements. — *Seeq Corp., Seattle, Wash.*
www.seeq.com

Manage safety risks with this improved software application

In May, this company released an improved version of its EcoStruxure Triconex Safety View, the industry's first dual safety- and cybersecurity-certified bypass and alarm management software application. EcoStruxure Triconex Safety View allows operators to see both the bypass status that impacts the level of risk reduction in place, as well as the critical alarms required to operate the plant safely when risks are high. And because the software has been certified by TÜV Rheinland as Security Level 1 (SL1) compliant per IEC 62443-4-2 and Systematic Capability 3 (SC3) compliant per IEC 61508 for use in safety-related applications up to Safety Integrity Level 3 (SIL3), it meets stringent requirements for safety, cybersecurity, risk reduction and continuous operation in the oil-and-gas, petroleum-refining, petrochemicals, power and other high-hazard, risk-intensive industries. Better bypass management, which EcoStruxure Triconex Safety View provides, can help companies better manage their safety risks, including risks that threaten the performance of their operations. — *Schneider Electric, Boston, Mass.*
www.se.com

New solution to simplify PPE selection

Especially during the time of COVID-19, personal protection equipment (PPE) PPE is vital. This company's PPE Selector software allows users to get clear and accurate guidance and instructions on the proper protective equipment. Every year, preventable incidents caused by workers not using the proper PPE lead to scores of workplace-related incidents and near-misses. Injuries are costly for employers, too. The new PPE Selector module for SpheraCloud is said to be the first Software as a service-based solution that automatically displays a list of recommended PPE based on the characteristics of the work. Key features include: fully configurable lists for recommended PPE, based on regulatory and in-house requirements; pictures of recommended PPE for easy identification and improved compliance; the ability to specify PPE at multiple stages of the permit-to-work lifecycle and to print or display the proper procedures and required PPE. — *Sphera Solutions, Inc., Chicago, Ill.*
www.sphera.com

New release for data analysis and graphing software

In May, this company released Origin and OriginPro 2021b. This latest version of software application (app) adds over 100 new features, apps and improvements, further enhancing ease-of-use, graphing, analysis and programming capabilities. OriginPro 2021b offers further enhancements to embedded Python support. Users can define Python functions in the Fitting Function Builder and Peak Analyzer, as well as run Python script directly from a button placed on a worksheet, matrix, or graph. Intellisense support has been added in the Python Console and Set Values dialog and embedded python script can now access curve fitting as well as analysis reports, metadata, and trees. A set of greatly enhanced features for NetCDF-based climate data graphing and analysis is available in this latest version. — *OriginLab Corp., Northampton, Mass.*
www.originlab.com

Support for complex data and cloud-to-edge integrations

The latest release of HighByte Intelligence Hub version 1.4 is an Industrial DataOps solution enabling manufacturers to streamline their data architecture and reduce time to deploy new systems. The software supports open standards and provides operations technology (OT) teams with the flexibility to merge, prepare, and deliver industrial information to and from IT systems without writing code. With its latest release, HighByte Intelligence Hub now supports complex, multi-value sets of data, a broader range of disparate data sources, flow consolidation, and additional security features. The latest release includes support for complex data sets that can be processed through HighByte Intelligence Hub's modeling engine, transforming and contextualizing information at high volumes. — *HighByte, Inc., Portland, Maine*
www.highbyte.com

Software update introduces tube-assistant feature

New software for the design of shell-and-tube heat exchangers has been further enhanced after its first update introduced a new Tube Assistant feature, making more information instantly accessible to users during the design process. AHED (Advanced Heat Exchanger Design) was officially launched in December 2020 and has been specifically designed to bring the latest theories and design techniques to a wide group of potential users, from students and academics through to industrial engineers and system designers. One of the key features of the collaborative, cloud-based AHED system is its database of 2,000 different fluids, meaning that key property parameters are available to users without need to look things up outside of the system. In January, a new AHED system update introduced another database in the form of the Tube Assistant. Updated versions of AHED now feature a "magic wand" symbol in the geometry section of the program. Clicking on this opens the new Tube Assistant feature, which contains details of different tube dimensions, including those commonly used for heat exchangers, as well as standard ISO, ANSI, and millimeter metric tube types. Fields in the table correspond to a specific tube outer diameter and wall thickness. Selecting the appropriate field then allocates these dimensions to the shell, inner tube, or nozzle in the current AHED project as required. — *AHED, Lorquí (Murcia), Spain*

www.hrs-ahed.com

Machine learning for improved operator performance

In June, this company introduced the addition of Operator Advisor to its Experion Highly Augmented Lookahead Operations (HALO) suite. This powerful software solution enables plant owners to objectively measure gaps and drive operator effectiveness to the next level. This market-first solution presents users with a consolidated scorecard of enterprise automation utilization and recommended steps to address performance-related gaps. The solution uses machine learning (ML)-powered analytics to gather insights from enterprise data sources, such as distributed control systems (DCS), and funnel those insights into dashboards. These dashboards can provide operations managers and supervisors with a clear and complete view of operator performance and improvement opportunities. By understanding how operator actions, inactions and workload levels contribute to optimal production, organizations can develop targeted training programs, make strides toward autonomous operations and build process resilience — all of which can help them better compete in the digital age. HALO Operator Advisor will be available in October 2021. — *Honeywell Process Solutions, Houston*

www.honeywellprocess.com ■

Gerald Ondrey

ystral

A new dispersing system for slurry production

The new Batt-TDS series of powder-dispersing systems (photo) is designed for the development and industrial production of electrode slurries for lithium-ion batteries. The platform offers crucial benefits, compared to existing technologies. The Batt-TDS handles diverse materials by combining multiple functions of several machines into a single core system. At R&D scale, compared to planetary mixers, which require hours of mixing to accomplish dispersion, the Batt-TDS can complete the entire process in a few minutes, enabling faster R&D cycles. Dispersion itself requires only milliseconds as components pass through its inline process chamber. At production scale, this translates to greater than ten-times higher productivity than conventional technologies and twice that of available extruders, says the company. The product range includes a 12-L unit for rapid formulation and process screening, and production systems for throughputs greater than 5,000 L/h. — *ystral GmbH, Ballrechten-Dottingen, Germany*
www.ystral.de

Bonomi North America

Explosion-proof automated V-ball valve packages

This company has introduced what is said to be industry's first explosion-proof electric-actuated stainless-steel two-piece V-ball packages. They are available in sizes ½ to 2 in. NPT. The new M8E700076V36-V6-V9 series electric actuated V-ball valve (photo) is said to offer precise proportional control in the smallest total dimensional envelope in the industry. This is due to the low-torque design of the 700076V stainless-steel V-port ball valve with 23% carbon-filled and 2% graphite-filled seats. The valve also incorporates dual Viton O-ring stem seals for long-lasting leak-free performance over an operating temperature range of –4 to 366°F. Pressure ratings are 1,000 psi (water, oil or gas) and 150 psi (steam). The valves are factory-assembled with the company's EXM Series electric actuator. — *Bonomi North America, Charlotte, N.C.*
www.bonominorthamerica.com

Gebr. Lödige Maschinenbau

High-shear granulator for compacting powdery foodstuffs

This company has developed a granulator (photo) designed for compacting bulk goods, such as tea, cocoa or coffee. It is based on the mixing granulator type MGT, a vertical system for mixing and granulation of powders and granules. A specially developed compaction tool rotates in the cylindrical mixing vessel at a close distance from the vessel wall and base to achieve the necessary bulk density and a homogeneous mixing quality. In addition, the mixing vessel is equipped with a cooling double jacket to ensure that the full aroma of the material is retained. The product can be flavored in accordance with the recipe parameters directly in the processing vessel of the Mixing Granulator. This process can be carried out manually or automatically. The machine requires only three minutes to mix and compress, for instance, one batch of ground coffee. — *Gebr. Lödige Maschinenbau GmbH, Paderborn, Germany*
www.loedige.de

Gardner Denver High Pressure Solutions

A 1,000-gal/min pump for horizontal drilling

The new GD 800HDD pump (photo) has an extremely high flowrate of more than 1,000 gal/min, making it suitable for the most demanding horizontal directional drilling (HDD) projects. Its light weight eases transportation between work sites and its extremely high rod-load rating of 53,000 lb ensures the pump is tough and long lasting, says the manufacturer. The pump is also designed to operate at a slow run speed, delivering the same output, flow, and pressure as faster pumps with less violent actions, wear and friction. By delivering fewer strokes, consumable life is extended. The pump is qualified as maxi-rig pump, and can provide a suite of options to the HDD industry when tunneling under rivers and roads and laying sewerage systems, water pipes, fiber-optic lines and pipelines. — *Gardner Denver (GD) High Pressure Solutions, Houston*
www.gardnerdenverpumps.com

Remote I/O IS1+ as an edge gateway for Zones 1 and 2

Alongside its proven remote input/output (I/O) functionality, IS1+ (photo) is now also available for use as an edge gateway with a connection via OPC UA and optional integrated signal pre-processing. In this process, all diagnostics and device data are transmitted parallel to the supported communication protocols Profibus DP, ProfiNet, EtherNet/IP or Modbus TCP via OPC UA to superordinate systems, such as aggregation servers or cloud applications. This means that IS1+ can be used in modern system concepts such as NAMUR Open Architecture (NOA) for monitoring and optimization functions using the second channel, and enables the use of these concepts in hazardous areas in Zone 1. For brownfield systems in particular, which often operate using Profibus DP, IS1+ offers a simple migration path: While process control is still performed via Profibus, all additionally available data from the system and connected field devices is transmitted via a second channel with Ethernet and OPC UA. — *R. Stahl, Waldenburg, Germany*

www.r-stahl.com

R. Stahl

Certify cables with this hand-held device

The new WireXpert 500 cable tester (photo) targets copper cabling up to Cat 6A standards. With its modular concept and unique licensing system, the WireXpert 500 is a versatile, cost-effective tool for cable system certification in office environments, industrial settings, laboratories and data centers. By enabling cable certification up to Cat 6A only, the WireXpert 500 fits over 95% of contractor requirements. Contractors can also easily upgrade WireXpert 500 units to certify copper cabling through Cat 8 or fiber optic cabling. The device features the Dual Control System, which equips both local and remote devices with a main processor and color LCD screen. These features reduce the amount of walking a single user must do during troubleshooting, improving the testing efficiency for smaller, one-person testing projects. — *Softing Inc., Knoxville, Tenn.*

itnetworks.softing.com/us

Softing

UL-rated pressure switches for explosive environments

The new 703-U and 703-UJ Series of UL-rated, explosion-proof pressure switches (photo) are suitable for gaseous or liquid fluid systems in hazardous applications, including offshore exploration, petrochemical processing and oil-and-gas pipelines. The 703-U and 703-UJ Series have a corrosion-resistant stainless-steel construction and UL ratings for hazardous locations, including Class 1: Division 1, Groups A, B, C, D, as well as Class 2: Groups E, F, G. Units also feature high overpressure capabilities, a NEMA Type 7 explosion-proof rating and rugged piston design, enabling these switches to withstand high pressure spikes, shock and vibration. The 703-U/UJ Series cover a pressure range: from 6 to 5,000 psi and a temperature range of –40 to 180°F. — *Sigma-Netics, Inc., Morristown, N.J.*

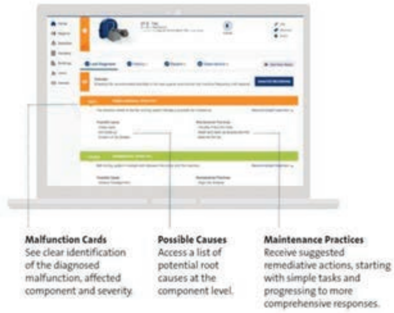
www.sigmanetics.com ■

Gerald Ondrey

Sigma-Netics

5TH ANNUAL CONNECTEDPLANT CONFERENCE
Harnessing Digital Tools to Drive Success


Seeq Corp.



Grundfos Pumps Corp.


TrendMiner US

Global digitalization professionals will convene in Austin, Tex. for the 2021 Connected Plant Conference (www.connectedplantconference.com), which is being held August 30–Sept. 2. The event will cover all aspects of the industrial internet of things (IIoT), and its enabling technologies, including machine learning (ML), artificial intelligence (AI) and augmented and virtual reality.

Important IIoT applications and implementation best practices for the chemical process industries (CPI) will be covered in great detail in presentations by a wide variety of industry experts from companies including Eastman Chemical, ExxonMobil, Evonik, Mitsubishi, Google, Black & Veatch, Lonza, BP and more. This show preview highlights some of the advanced technologies that will be showcased at this year's Connected Plant Conference.

A full-service IIOT platform that supports flow-control equipment

RedRaven is an IIoT services platform that enables operators to digitalize operations with full-spectrum wireless monitoring, analytics and managed-engineering services. The RedRaven platform supports any flow-control equipment, regardless of manufacturer. The platform's intelligent fluid-motion insights improve plant resilience with agile protocols that serve to predict, act and protect. Available with wireless or wired options based on applications, the platform includes sensors that are placed on industrial equipment and gateways that collect data from assets and then transmit them to the cloud with a secure, data-encrypted technology. — *Flowserve, Corp., Irving, Tex.*
www.flowserve.com

New software features facilitate machine-learning initiatives

The new R52 release of this company's software platform (photo) offers new features that support the use of ML innovation in process manufacturing organizations. These features enable users to deploy their own or third-party ML algorithms into the advanced analytics applications used by frontline process engineers and subject matter experts, thus scaling the efforts of a single data scientist to many operational employees. New capabilities include add-on tools, display panes and user-defined functions, each of which extend the predictive, diagnostic and descriptive analytics capabilities. With R52, users will also be able to schedule Seeq Data Lab notebooks to run in the background. In addition to Seeq Data Lab support for ML code and libraries, the platform also enables access to the Seeq/Python library via third-party ML solutions, including Microsoft Azure, Amazon SageMaker and open-source offerings, such as Apache Anaconda. — *Seeq Corp., Seattle, Wash.*
www.seeq.com

Advanced machine-health platform for rotating equipment

This company's AI-powered machine-health platform, Grundfos Machine Health (GMH; photo), empowers users to convert their data into meaningful actions aimed at optimizing maintenance planning and improving reliability. GMH can be installed on nearly any piece of stationary rotating equipment to ensure complete site coverage. The platform's advanced wireless sensors are installed non-invasively at all bearing points on the machine. Data is transferred to an ISO 27001-certified, secure cloud platform where a robust algorithm uses measurements of vibration, temperature and magnetic flux to detect the slightest variation in equipment's optimal performance. The variant is then translated into actionable tasks that help maintenance teams prioritize their workload and prevent costly failures. — *Grundfos Pumps Corp., Brookshire, Tex.*
us.grundfos.com

Next-generation productivity through self-service analytics

This company's intuitive, web-based self-service analytics platform (photo) enables rapid visualization of time-series based process

and asset data. Using this self-service, advanced-analytics solution supports improving an organization's key performance indicators (KPIs), while also reducing costs. Classic model-based analytics require data-science expertise and can often be time consuming. Enabling more users to access advanced analytics decreases "time-to-insight." This democratization of analytics supports people with a deep understanding of the process to improve the performance of the plant. The platform analyzes both time-series data and contextual data. Users can find relevant data, identify trends and create actionable information to solve production issues. They can also troubleshoot problems and monitor processes and assets in real-time to make better decisions, faster. — *TrendMiner US, Houston*

www.trendminer.com

Smart predictive analytics for heat-transfer-fluid maintenance

Fluid Genius is a new predictive analytics tool for heat-transfer-fluid (HTF) life expectancy that uses AI algorithms built around HTF sample analysis data. The tool is designed to provide recommendations for extending fluid life and maintaining HTF systems. Fluid Genius generates a fluid condition score, a unique measure of the overall fluid condition, as well as notifications about fluid trends and customized recommendations for proactive maintenance actions. These could include system venting, inert-gas blanket system installation and inspection, fluid replacement, the implementation of side-stream filtration and alerts for possible contamination. — *Eastman Chemical Co., Kingsport, Tenn.*

www.eastman.com

Cloud-based APM merges modeling and analytics

The Forge Asset Performance Management (APM) platform goes beyond traditional machine monitoring and data gathering by merging machine modeling with modern cloud analytics. Digital twins developed in this platform predict machinery availability, drill to the root cause of inefficient machine operation and bring order to reliability and maintenance planning. Forge APM deploys rapidly through a variety of standard asset libraries and tools to integrate data sources quickly. To achieve peak asset performance and maximize machinery uptime, Forge APM supports greater enterprise asset management, even where pre-existing monitoring systems are already installed. — *Honeywell International Inc., Charlotte, N.C.*

www.honeywell.com

Explainable machine learning for manufacturing optimization

This company's software platform aims to make manufacturing more efficient through explainable machine learning. With this easy-to-use software, factory personnel can optimize production and address root causes of quality issues, with no data-science experience required. Once deployed, models offer real-time optimization suggestions that constantly learn from the latest production data. Visual dashboards allow results to be shared with operations teams, so models can be scaled to other plants within weeks. A highlight of this solution is the ability to virtually replicate multi-stage batch processes in the software. With this functionality, users can model complex interactions between stages of batch processes with a high degree of accuracy, providing key data for decision-making. — *Fero Labs, New York, N.Y.*

www.ferolabs.com ■

Mary Page Bailey

Time and Length Scales of Mixing: The Macro Scale

Successfully scaling up a mixing process involves understanding several important timescale parameters that can impact chemical reactions and equipment performance

R. K. Grenville, J. J. Giacomelli, B. A. Boyer and S. J. Johnson
Philadelphia Mixing Solutions, An SPX FLOW Brand

IN BRIEF

Many industrial processes are defined by rates. For example, rates of mass and heat transfer, rates of reaction and rates of addition to a reactor. Even a batch process can be described in terms of a rate — the number of batches to be completed in a day. If mixing is required to achieve the process result, then the rate of mixing must often be related to the process rate. In reaction engineering, the ratio of mixing rate to reaction rate is the Damkohler number [*1*]. It is also useful to consider the inverse of the rate, which is a timescale. Comparison of rates or timescales enables an engineer to determine which is likely to dominate the process and identify when interactions are likely to occur. Understanding the role of mixing and quantification of these rates often plays an important role in successful process design and scaleup.

There is a spectrum of scales to consider depending on the nature of the process in question. There are five timescales, with associated length scales, of interest in mixing processes, which are defined in Table 1. Note that in this article, the first three timescales, which take place at the scale of the vessel, and their associated length scales, are reviewed.

Mean residence time

Figure 1 shows a sketch of a continuous stirred-tank reactor (CSTR) with volume V and flowrate Q. The mean residence time is defined as the operating volume of the vessel divided by the flowrate through it. It is the average time that a packet of fluid spends in the vessel. In principle, some of the entering fluid will immediately travel to the outlet and leave, while some will remain in the vessel for an infinite time. The variation in these times is described by the residence-time distribution [*2*].

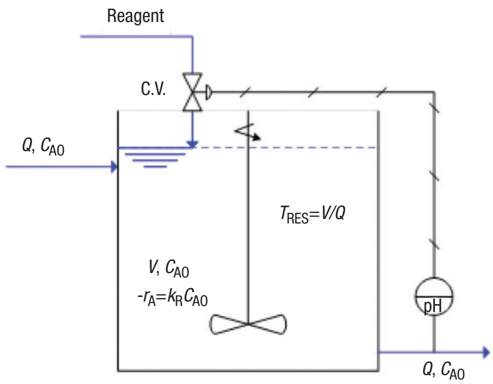


FIGURE 1. A continuous stirred-tank reactor with feedback pH control is illustrated

This analysis assumes that the vessel contents are "perfectly back-mixed," which means that the composition of the fluid leaving the vessel (C_{AO}) is equal to the average composition inside it. In addition, it assumes that the feed stream entering the vessel is instantaneously mixed with the contents. This is a key assumption in the calculation of

TABLE 1. TIME AND LENGTH SCALES IN MIXING

Scale	Decription
1. Mean residence time (or space time)	In a continuous stirred-tank reactor (CSTR), this is simply the operating volume divided by the flowrate through the vessel.
2. Circulation time	This is the time taken, on average, for a packet of fluid to travel from the impeller, around the vessel and back to the impeller again
3. Blend time	This is the time taken for the material added to a vessel to be blended to a desired degree of homogeneity with all the vessel contents. The required degree of homogeneity will be determined by a description of the process, or the process result
4. Meso-mixing timescale	This is associated with the time taken to disperse the feed entering a semi-batch or continuous reactor and is particularly important in the understanding of the role of mixing in fast, competitive or parallel chemical reactions
5. Micro-mixing timescale	This is associated with the time taken for the smallest turbulent eddies to shrink down to the Kolmogorov length scale where they lose their structural identity and their kinetic energy is dissipated as heat. This occurs when the Reynolds number of the eddies is unity and the inertial and viscous stresses are in balance

conversion in a CSTR [3]. For a first-order reaction, the conversion (X) can be calculated using Equation (1):

$$X = 1 - \frac{1}{1 - k_R \tau_{res}} \quad (\mathbf{1})$$

This is also a key assumption in the design of pH-control systems. Figure 1 also shows a feedback pH-control scheme with the pH of the fluid leaving the vessel being measured and with its value fed back to adjust the position of the reagent feed valve. If the assumption of perfect back-mixing is not valid, the system will be out of control and the pH will oscillate around the desired setpoint. This is particularly difficult if a strong acid is being neutralized with a strong base, and vice versa [4].

For this assumption to be true, the incoming feed must be instantaneously blended with the fluid inside the vessel, which is physically impossible. But even though instantaneous blending is not realistic, under certain circumstances, the assumption of perfect back-mixing can be made valid.

A rule of thumb has been proposed in Ref. 5 relating the mean residence time to the batch blend time, θ. This rule of thumb states that the contents of the continuous reactor can be assumed to be perfectly back-mixed if the following statement is true:

$$\frac{\tau_{res}}{\theta} > K, \text{ where } K \approx 10$$

Ref. 6 provides measurements of residence-time distribution for three impellers over a range of flowrates and, hence, residence times. The authors concluded that the degree of bypassing and stagnation (dead zone behavior) increased as the feedrate increased, but were unable to correlate their conclusions to any ratio of timescales.

The authors of Ref. 7 also carried out similar experiments and concluded that the degree of bypassing observed was dependent on the ratio of the momentum generated by the impeller to the momentum of the feed jet, M_{jet}. The momentum of the feed jet is given in Equation (2):

$$M_{jet} = \rho \, Q_{feed} \, U_{feed} \propto \frac{Q_{feed}^2}{D_{feed}^2} \quad (\mathbf{2})$$

And the momentum generated by the impeller is defined in Equation (3):

$$M_{imp} = Mo \, \rho \, N^2 D^4 \quad (\mathbf{3})$$

where Mo is the impeller's Momentum number. The Momentum number can be calculated from Equation (4) in terms of the impeller's Flow number [8]:

$$Mo = 1.43 \, Fl^2 \quad (\mathbf{4})$$

Jones and others [7] concluded that in cases where $M_{imp} \geq 100 M_{jet}$, flow generated by the impeller dominates the flow within the vessel and perfect CSTR behavior could be achieved. If bypassing is being observed in an existing CSTR, the residence-time distribution (RTD) can be moved toward "perfect behavior" by reducing the momentum of the feed jet. Since the flowrate, Q_{feed}, is fixed by process requirements, the jet momentum can be reduced by increasing the diameter of the feed pipe, D_{feed}.

Another consideration in the design of CSTRs is the location of the inlet and outlet to the vessel. The general rule is that the outlet should be located far from the inlet [9]. Time-dependent computational fluid-dynamics (CFD) techniques, such as large-eddy simulation, have been successfully applied to investigate issues relating to both the momentum ratio and inlet and outlet positions in CSTR operation [10, 11].

Velocity and circulation time

One of the common scaling rules for sizing agitated vessels is constant torque per unit volume. Torque is the product of a force and a distance, so it has the same units of measurement as work or energy. This means that torque per volume can be thought of as the work that is done, or energy

NOMENCLATURE

A	Vessel cross-sectional area	m^2
C_A	Concentration of A	kmol m^{-3}
D	Diameter of impeller	m
D_{feed}	Diameter of feed pipe in CSTR	m
Fl	Flow number (= Q_{imp} / ND^3)	
H	Liquid depth	m
k_R	Reaction rate constant	s^{-1}
Mo	Momentum number (= $M_{imp} / \rho N^2 D^4$)	-
M_{imp}	Momentum of impeller discharge flow	kg m s^{-1}
M_{jet}	Momentum of feed jet in CSTR	kg m s^{-1}
N	Impeller rotational speed	rps
Po	Power number (= $P/\rho N^3 D^5$)	-
Q_{feed}	Flow rate of feed in CSTR	m^3 s^{-1}
Q_{imp}	Impeller pumping capacity	m^3 s^{-1}
Re	Reynolds number (= $\rho ND^2\mu$)	-
Re_B	Reynolds number at boundary between the turbulent and transitional regimes	-
S	Fluid specific gravity	-
T	Diameter of vessel	m
U_{BF}	Bulk fluid velocity	m s^{-1}
U_{feed}	Velocity of feed jet in CSTR	m s^{-1}
U_{tip}	impeller tip speed	m s^{-1}
V	Vessel volume	m^3
V_{EQ}	Equivalent volume	m^3
X	Conversion	-
α	Constant in correlation for blend time	-
β	Exponent in correlation for blend time	-
E	Energy input per mass	J kg^{-1}
$\bar{\varepsilon}$	Power input per mass	W kg^{-1}
Γ	Agitator shaft torque	Nm
ζ	Degree of homogeneity	%
η	Impeller pumping efficiency	kg J^{-1}
μ	Fluid viscosity	kg m^{-1} s^{-1}
θ	Blend time in batch system	s
ρ	Liquid density	kg m^{-3}
τ_{Circ}	Mean circulation time (V/Q_{imp})	s
τ_{Res}	Mean residence time in CSTR (V/Q_{feed})	s
Φ	Torque per mass	Nm kg^{-1}
Ψ	Torque per volume	Nm^{-2}

input, by the impeller to that volume of liquid. Therefore, torque can be used as a method for quantifying agitation intensity.

Connolly and Winter developed a design procedure that aimed to duplicate velocities at critical points in mixing vessels or create kinematic similarity [*12*]. This can be achieved by applying equal torque per volume. Hicks and others [*13*] proposed a scale of agitation, ranging from 1 to 10, where one unit on the scale corresponded to a bulk fluid velocity of 6 ft/min. The bulk fluid velocity, U_{BF}, is simply the flow generated by the impeller divided by the cross-sectional area of the vessel. So, for a cylindrical vessel, U_{BF} is determined by Equation (5):

$$U_{BF} = \frac{Q_{imp}}{A} = \frac{4}{\pi}\frac{Fl\,N\,D^3}{T^2} \quad \textbf{(5)}$$

The impeller tip speed is given by Equation (6):

$$U_{tip} = \pi N D \quad \textbf{(6)}$$

Equations (5) and (6) can be combined to give Equation (7) below:

$$U_{BF} = \frac{4}{\pi^2} Fl\, U_{tip} \left(\frac{D}{T}\right)^2 \quad \textbf{(7)}$$

The torque acting on the impeller shaft can be calculated from Equation (8):

$$\Gamma = \frac{Po\,\rho\,N^2D^5}{2\pi} \quad \textbf{(8)}$$

The torque per volume in a vessel where the liquid depth is equal to the vessel diameter ($H = T$) is given in Equation (9):

$$\Psi = \frac{2}{\pi^2} Po\,\rho\,(ND)^2 \left(\frac{D}{T}\right)^3 \quad \textbf{(9)}$$

One potential drawback of this approach is that the torque and torque per unit volume are proportional to the density of the fluid, so the torque per volume will be higher if the fluid is denser in order to achieve the same bulk fluid velocity. This is not an issue if the approach is being applied to scaleup, since the density of the fluid will be the same at both scales. However, it will be a problem if torque per unit volume or bulk fluid velocity are being used as the basis for design. Hicks and others [*13*] proposed using the "equivalent volume," which is the product of the fluid's specific gravity and volume. In that case, Equation (9) becomes Equation (10), where S is the fluid specific gravity and $\rho = S \times 1{,}000$.

$$\Psi_{Eq} = \frac{1}{2\pi}\frac{Po\,\rho\,N^2D^5}{SV} = \frac{1}{2\pi}\frac{Po\,\rho\,N^2D^5}{V_{Eq}} \quad \textbf{(10)}$$

Alternatively, the agitation intensity could be expressed in terms of torque per mass or specific energy input, as shown in Equation (11):

$$\Phi = \frac{1}{2\pi}\frac{Po\,\rho\,N^2D^5}{\rho V} = \frac{1}{2\pi}\frac{Po\,N^2D^5}{V} \quad \textbf{(11)}$$

Equations (6) and (11) can be combined into Equation (12):

$$\Phi = \frac{2}{\pi^4} Po\, U_{tip}^2 \left(\frac{D}{T}\right)^3 \quad \textbf{(12)}$$

Equations (7) and (12) can then be combined into Equation (13):

$$U_{BF} = \left(8\,\frac{Fl^2}{Po}\frac{D}{T}\Phi\right)^{1/2} \quad \textbf{(13)}$$

So, the bulk fluid velocity is proportional to the square root of the torque per mass, but the actual relationship also depends on the type of impeller, through its power and flow numbers, and its diameter relative to the vessel diameter, or D/T ratio.

Once the bulk fluid velocity has been estimated, the internal circulation time of the fluid will be proportional to the path taken by the packets of fluid divided by the velocity of the packets. The length of the path will be proportional to a length scale of the vessel, the diameter, as shown in Equation (14):

$$\tau_{Circ} \propto \frac{T}{U_{BF}} \quad \textbf{(14)}$$

This shows that the consequence of scaling up with constant torque per (equivalent) volume or mass is that the circulation time increases in proportion to the scaleup factor.

An alternative way to examine this relationship is to define the circulation time in terms of the operating volume and pumping capacity of the impeller, as shown in Equation (15):

$$\tau_{Circ} = \frac{V}{Q_{IMP}} = \frac{\pi}{4}\frac{T^3}{Fl\,N\,D^3} \quad \textbf{(15)}$$

Equation (16) below shows Equation (15) in terms of the impeller tip speed:

$$\tau_{Circ} = \frac{\pi^2}{4\,Fl\,U_{Tip}}\left(\frac{T}{D}\right)^2 T \quad \textbf{(16)}$$

This approach also shows that, when scaling up at constant tip speed, the circulation time increases in proportion to the scale factor. The larger the impeller diameter, the shorter the circulation time because a larger-diameter impeller acts as a more efficient pump [*14*]. Scaling up at constant torque per volume and tip speed (with geometrical similarity) will result in the reduction of power input per unit mass. The rotational speed will reduce as the impeller diameter increases, so the power per volume will decrease in proportion to the reduction in speed or increase in scale.

Equation (15) shows that if equal circulation time is required on scaleup (with geometrical similarity), the agitator must operate at the same rotational speed at the large and small scales. The power drawn by an impeller is given in Equation (17):

$$P = Po\,\rho\,N^3D^5 \quad \textbf{(17)}$$

The power input per mass of fluid is given in Equation (18):

$$\bar{\varepsilon} = \frac{4}{\pi} Po\,N^3D^2 \left(\frac{D}{T}\right)^3 \quad \textbf{(18)}$$

As a result, scaling up at constant impeller speed and geometry leads to an infeasible increase in power input and power per mass, so this approach is rarely taken.

Scaleup rules, such as constant tip speed, torque per volume, power

per mass or constant bulk-fluid velocity allow the engineer to size an agitator without necessarily having a good understanding of the role mixing has on the outcome of their process [*15*]. Most mixing processes are promoting a change in the contents of the vessel and the success of the process will be determined, to some extent, by the rate at which this change occurs. If the rate-limiting process can be identified, then the goal of scaleup should be to match the rate of mixing to the rate-limiting step, although care must be taken to determine whether the rate-limiting step changes with scale.

Blend time

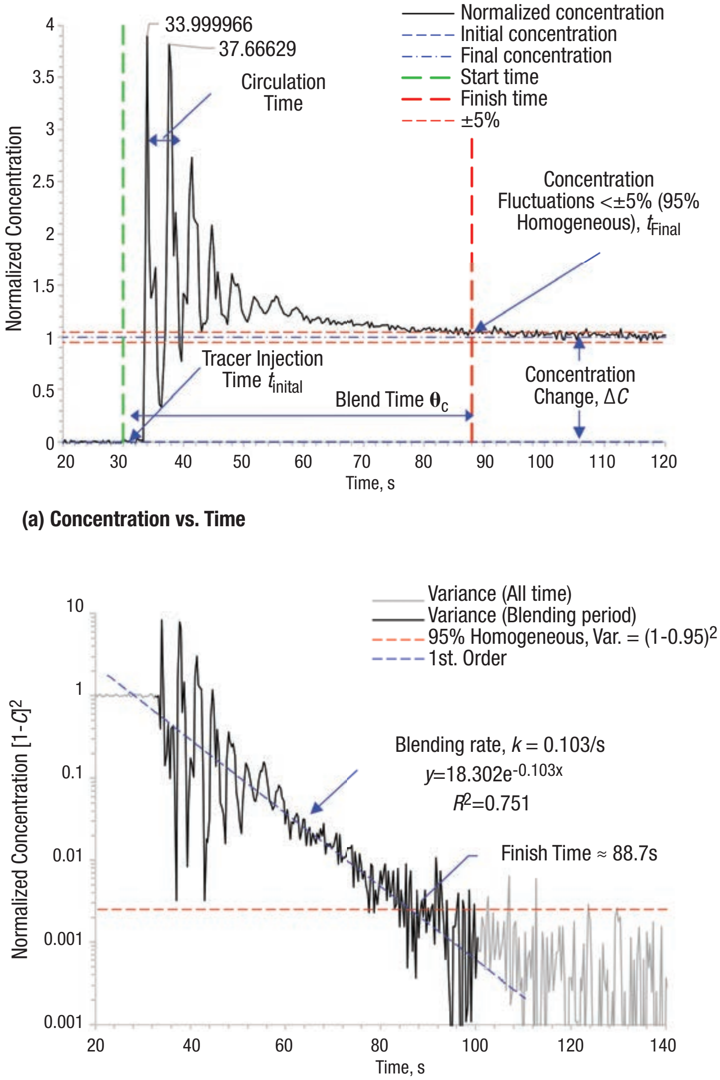
Blending rate is defined as "the rate that concentration differences are reduced by large-scale circulation and convective flow down to a selected level of variation everywhere in the whole vessel [*16*]." The blend time is inversely proportional to this rate. The rate of blending is proportional to the rotational speed of the impeller and, in the turbulent regime, the product of blend time and impeller speed is a constant. This value represents the number of revolutions that the impeller must make to reach the desired level of variation or homogeneity. It is dependent on the impeller type and its size.

There have been many studies on blending using a variety of experimental methods, including the following:

1. Adding acids and bases and recording the time for color change with a pH indicator [*17*, *18*, *19*].
2. Adding tracer of hot fluid and measuring temperature change [*19*, *20*, *21*].
3. Adding a concentrated brine tracer and measuring conductivity changes [*19*, *22*, *23*, *24*, *25*].

Landau and Procházka [*19*] compared all three methods and concluded that they are mutually consistent, so it is possible to reliably compare results measured with these techniques.

Figure 2a shows a typical conductivity trace for a blend-time experiment. In this experiment, the conductivity is recorded for about 25 s to establish the initial conditions and then the tracer is added, shown by the green vertical line. There is a short lag as the packet of tracer is carried to the probe and then there is a spike in the conductivity reading. The packet is carried away and the measured conductivity falls as the salt within the packet is diluted by the surrounding liquid. Eventually, the conductivity reaches a steady state and the vessel contents are homogeneous. The time taken to reach 95% homogeneity (conductivity fluctuations within ±5% of the final value) is shown by the vertical red line. An alternative method for extracting the blend time from the measurement is to plot the log of the variance in the conductivity measurement versus time, as shown in Figure 2b. This is especially useful when conductivity is measured with several probes, since the variance gives a measure of homogeneity for the whole vessel based on the individual probe responses [*24*]. The slope of the curve represents the mixing rate.



(a) Concentration vs. Time

(b) Variance vs. Time

FIGURE 2. The plot of conductivity versus time (a) shows the time taken to reach 95% homogeneity (the vertical red line). Alternatively, normalized variance versus time (b) is plotted when systems are using multiple conductivity probes, resulting in a measure of homogeneity for the whole vessel based on the individual probe responses. The slope of the plot represents the blending rate

Results are usually expressed by plotting the dimensionless blend time, which is the product of the measured blend time and the impeller speed, $N\theta$. This represents the number of revolutions that the impeller must make in order to achieve the desired level of variation or homogeneity. In the turbulent regime, the value of the dimensionless blend time is constant, and it depends on the type and size of the impeller. Figure 3 shows a plot of dimensionless blend time versus Reynolds number (Re) for two diameters of pitched-blade turbines measured in four vessels ranging from 1 to 9 ft in diameter. There are two regimes identified in Figure 3. In the turbulent regime, $N\theta$ is constant

TABLE 2: VALUES OF α AND β REPORTED BY VARIOUS AUTHORS

			Rushton		Pitched-blade		Propeller		Hydrofoil	
Authors	**Year**	**T/D**	α	β	α	β	α	β	α	β
Prochaka and Landau	1961	3–10	1.56	2.57	2.31	2.20	2.35	2.05	-	-
Shiue and Wong	1984	2–3	8.57	2.40	-	-	-	-	3.88	2.24
Grenville	1992	2–3	5.20	2.00	5.20	2.00	5.20	2.00	5.20	2.00
Strand and Hensel	2018	2–5	5.19	2.30	5.76	2.21	-	-	8.12	1.93

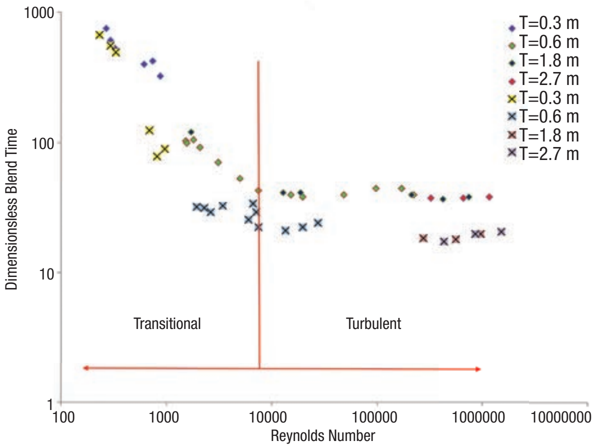


FIGURE 3. Dimensionless blend time (Nθ) is plotted against Reynolds number for pitched-blade turbines, 1/3 and 1/2 of the vessel diameter (T), measured at four vessel scales

and the value of the constant depends on the impeller type, through its power number, and the ratio of impeller to vessel diameters. At a certain Re value, the blending regime becomes transitional and *N*θ is inversely proportional to Reynolds number — which means that it is proportional to the fluid's viscosity.

The value of Reynolds number at the boundary (Re_B) between the regimes is dependent on impeller type and can be estimated from Equation (19) [*24*]:

$$Re_B = \frac{6,400}{Po^{1/3}} \quad \textbf{(19)}$$

The reason for this is the difference in power input by different impellers when compared at the same Reynolds number. For example, the power input by a Rushton turbine (*Po* = 5.0) will be approximately 15 times higher than the power input by a hydrofoil (*Po* = 0.3) at the same speed and diameter, and, therefore, Reynolds number. Khang and Levenspiel measured blend times for Rushton turbines and marine propellers and reported the same result [*23*].

Most authors agree that, in the turbulent regime (where $Po^{1/3}Re > 6,400$), the best correlation of their data is in the form given in Equation (20):

$$N\theta_\zeta = \frac{\alpha}{Po^{1/3}}\left(\frac{T}{D}\right)^{\beta} \quad \textbf{(20)}$$

The power number accounts for the effect of impeller type and the vessel to impeller diameter ratio, *T/D*, accounts for the impeller size. ζ represents the "selected level of variation" or degree of homogeneity required. For example, for 99% homogeneity, or a variation of ±1%, ζ = 99. Values of α and β found by various researchers are summarized in Table 2. The values of α vary, but the values of β generally fall within ±15% of 2.00.

To test the effect of these differences, the blend times predicted by the Grenville [*24*] and Strand and Hensel [*25*] correlations have been calculated for Rushton (*Po* = 5.0) and pitched-blade turbines (Po = 1.5) and a narrow-blade hydrofoil (*Po* = 0.3), since they used the same experimental technique. In each

TABLE 3. BLEND TIMES PREDICTED BY CORRELATIONS OF GRENVILLE *[24]* AND STRAND & HENSEL *[25]*

		Rushton	Pitched-blade	Hydro-foil
Power, hp		19.84	6.35	1.18
Grenville, s	θ	15.81	25.73	39.85
Strand and Hensel, s	θ	21.94	35.02	57.61

case, the impeller diameter is 36 in. and it operates at 100 rpm in a vessel that is 108 in. in diameter (*T/D* = 3). These results with the impeller power draw are summarized in Table 3.

While the blend-time predictions are in the same "ballpark," generally, the Strand and Hensel correlation predicts a blend time that is approximately 50% longer than Grenville's. Both used changes in conductivity to measure the blend time, and the difference in prediction is most likely due to the locations chosen for the conductivity probes. Strand and Hensel placed their probes much closer to the liquid surface than Grenville in a region where the mixing rate was slower. Even though there are differences in predictions made by the two correlations, the overall trends in terms of impeller type, *Po*, and size, *T/D*, are the same. Also, the blend time is the order of tens of seconds, which is very short compared to other process timescales, such as filling or emptying the vessel.

The degree of homogeneity measured in most experimental work is 95%. The reason for this is that as the degree of homogeneity becomes larger, the concentration fluctuations being detected are so small that they are lost in the background signal noise of the measurement equipment. The 95% blend time can be converted into a different degree of homogeneity because the approach to uniformity is exponential, since blending is a first-order process. The relationship between θ_{95} and θ_ζ is shown in Equation (21):

$$\theta_\zeta = \theta_{95}\frac{\ln(1-\zeta/100)}{\ln(1-0.95)} \quad \textbf{(21)}$$

So, for example, the blend time

for 99.99% homogeneity is three times longer than the blend time for 95%.

Blending and circulation

Equations (18) and (20) can be combined to express the blend time in terms of the power input by the impeller per mass of liquid, as shown in Equation (22):

$$\theta_{95} = \alpha \left(\frac{4}{\pi}\right)^{1/3} \bar{\varepsilon}^{-1/3} \left(\frac{T}{D}\right)^{(\beta - 5/3)} T^{2/3} \quad \textbf{(22)}$$

Equation (22) shows that when scaling up with constant power per mass with the same impeller type and geometry (meaning α, β and T/D are constant), the blend time will increase by the scale factor raised to the 2/3 power.

The values of ß, shown in Table 2, are always greater than 5/3 and the exponent on T/D is positive, so Equation (22) also shows that a larger-diameter impeller will be more efficient, achieving a shorter blend time for a given power input per mass.

Equally, Equations (15) and (18) can be combined to express the circulation time in terms of the power input by the impeller per mass of liquid, as shown in Equation (23):

$$\tau_{Circ} = \left(\frac{\pi}{4}\right)^{2/3} \frac{Po^{1/3}}{Fl} \bar{\varepsilon}^{-1/3} \left(\frac{T}{D}\right)^{4/3} T^{2/3} \quad \textbf{(23)}$$

Therefore, operating at constant power input per mass, the circulation time will also increase by the scale factor raised to the 2/3 power, but it is more sensitive to the T/D ratio with an exponent of 4/3.

Circulation versus blend time

The ratio of blend to circulation time is a measure of how many times the vessel contents must be turned over in order to achieve the desired degree of homogeneity. Equations (15) and (20) can be combined to give Equation (24):

$$\frac{\theta_{95}}{\tau_{Circ}} = \frac{4}{\pi} \alpha \frac{Fl}{Po^{1/3}} \left(\frac{D}{T}\right)^{(3-\beta)} \quad \textbf{(24)}$$

Using values of $\alpha = 5.2$ and $\beta = 2.0$ from Grenville [*24*] for 95% homogeneity, Equation (24) becomes Equation (25):

$$\frac{\theta_{95}}{\tau_{Circ}} = 6.62 \frac{Fl}{Po^{1/3}} \frac{D}{T} \quad \textbf{(25)}$$

Equation (25) predicts that this ratio will be smaller for a small-diameter impeller. For a pitched-blade turbine (Po = 1.50; Fl = 0.80 [*14*]), the blend time will be equal to the circulation time when D/T = 0.22 and for a Rushton turbine (Po = 5.00; Fl = 0.65 [*14*]) when D/T = 0.40. So, using this definition of circulation time shows that, if the D/T ratio is less than these values, the vessel should become homogeneous before the vessel contents have been turned over once.

Holmes and others [*26*] and Roberts and others [*27*] have measured the circulation time experimentally and both found that, for a Rushton turbine, the circulation time is proportional to T/D squared. Roberts and others [*27*] also defined the relationship given in Equation (26):

$$\tau_{Circ} = \frac{0.64}{N} \left(\frac{T}{D}\right)^2 \quad \textbf{(26)}$$

Combining Equations (20) and (26) results in Equation (27):

$$\frac{\theta_{95}}{\tau_{Circ}} = 1.56 \frac{\alpha}{Po^{1/3}} \left(\frac{D}{T}\right)^{(2-\beta)} \quad \textbf{(27)}$$

Again, taking $\alpha = 5.2$ and $\beta = 2.0$ from Grenville [*24*] and a Po of 5.00 for a Rushton turbine [*14*], Equation (27) simplifies to Equation (28):

$$\frac{\theta_{95}}{\tau_{Circ}} = 4.74 \quad \textbf{(28)}$$

Roberts and others also measured the circulation time for pitched-blade turbines but did not report a correlation of this data set. They did provide a table of data, which can be regressed to give Equation (29):

$$N \tau_{Circ} = 0.38 \left(\frac{T}{D}\right)^{3.05} \quad \textbf{(29)}$$

If the exponent is rounded off to 3.00, the pre-constant changes to 0.40. So, for pitched-blade turbines with Po = 1.50, Equation (30) applies:

$$\frac{\theta_{95}}{\tau_{Circ}} = 11.4 \frac{D}{T} \quad \textbf{(30)}$$

It is not clear why the ratio of blend to circulation times has a different dependency on the impeller to vessel diameter ratio for Rushton and pitched-blade turbines, although the primary flow that they generate is significantly different. The Rushton turbine generates a radial jet that splits when it reaches the vessel wall with flow loops created above and below the impeller. On the other hand, pitched-blade turbines generate an axial jet with a single flow loop.

Final thoughts

The macro-timescales of mixing in a well-designed stirred tank are on the order of tens of seconds and the process can be considered to be well-mixed under most circumstances, since this timescale will be short compared to other steps, such as filling and emptying the contents.

For CSTR design, a good first-pass analysis can be conducted based on the method described here, especially if the impeller-to-feed-momentum ratio is considered. Large-eddy simulation CFD models can also be reliably used to assess CSTR performance [*10*].

If the timescale of a chemical reaction is long compared to the blend time, for instance on the order of several minutes, the reactants will exist in a well-mixed environment and the yield or selectivity of the reaction will be governed by the reaction kinetics. Conversely, if the rate of reaction is faster than the rate of mixing, the local conditions at the feed point will determine the selectivity. Essentially, the reaction is over before the vessel contents are blended, and this must be taken into account in the design of the mixing equipment. ■

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Hydrogen Piping Systems: Mitigating Pitfalls by Design

This overview presents guidance for the safe design of piping systems that are used for the distribution of hydrogen gas

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Hydrogen gas is a very volatile fluid that has a high propensity to leak. This is a very dangerous and lethal combination of tendencies, a volatile fluid that is difficult to contain. These are tendencies that need to be taken into consideration when selecting material, gasketing and sealing, as well as the design characteristics of such a system. These topics regarding H_2 gas distribution are the focus of this discussion, not the manufacture of H_2, H_2 in its liquid state, nor slush H_2 (see sidebar on p. 35).

FIGURE 1. Hydrogen pipelines are a common sight at petroleum refineries

Properties of H_2

The following are a few key points of hydrogen gas and H_2-air mixtures that are helpful to know. There are two modes in which H_2 gas will burn: by deflagration and by detonation.

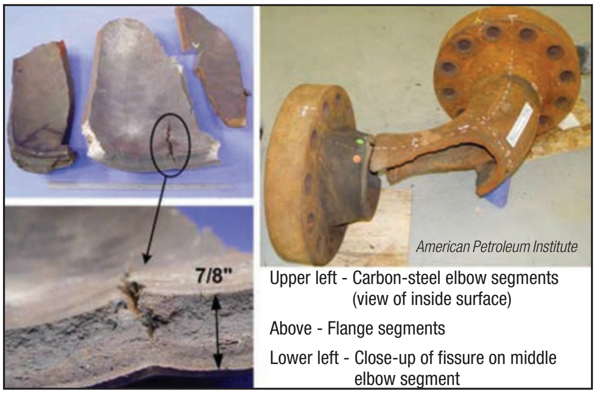
Deflagration. Deflagration is the ordinary mode of burning in which the flame travels through the mixture at subsonic speeds. As an example, this happens when a free cloud of H_2-air mixture is ignited by a small ignition source. In such a case the flame will travel at a rate anywhere from ten to several hundred feet per second. The rapid expansion of hot gases produces a pressure wave whose force is in direct proportion to the size of the cloud. The force of the pressure wave can be strong enough in some cases to damage building structures and other objects in its path and cause injury to personnel.

Detonation. With a detonation, the flame and the shock wave travel through the mixture at supersonic speeds. The pressure ratio across a detonation wave is considerably greater than that found in a deflagration. The hazards to personnel, structures and nearby facilities are greater in a detonation due to the added force. A detonation can build up from an ordinary deflagration when ignited in a confined area. In such a confined area, ignition can be caused by a minimal energy source. But detonation of a H_2-air mixture in an unconfined area requires a more powerful ignition source.

The pressure ratio across a detonation wave in a H_2-air mixture is about 20. At atmospheric pressure, a ratio of 20 equals 300 psi. When this wave of pressure strikes a fixed object the pressure ratio increases to between 40 and 60. This is due to the pressure wave bouncing back on itself from a fixed obstacle.

Propensity to leak. Due to its low viscosity and low molecular weight, gaseous H_2 has a high propensity to leak, and even permeate through or into various materials.

H_2 gas is eight times lighter than natural gas, 14 times lighter than air, 22 times lighter than propane and 57 times lighter than gas-



Upper left - Carbon-steel elbow segments (view of inside surface)

Above - Flange segments

Lower left - Close-up of fissure on middle elbow segment

FIGURE 2. Shown here is the damage caused by high-temperature hydrogen attack

TABLE 1. CODES, STANDARDS AND REGULATIONS RELATED TO HYDROGEN PIPING

Codes and Standards	Titles
29 CFR 1910.103	Hydrogen
API 940	Steel Deterioration in Hydrogen
API 941	Steels for Hydrogen Service at Elevated Temperatures and Pressures in Petroleum Refineries and Petrochemical Plants
ASME B31.3	Process Piping
ASME B31.12	Hydrogen Piping and Pipelines
ASTM B-849	Standard Specification for Pre-Treatments of Iron or Steel for Reducing Risk of Hydrogen Embrittlement
ASTM B-850	Standard Guide for Post-Coating Treatment of Iron or Steel For Reducing Risk of Hydrogen Embrittlement
ASTM F-1459	Test Method for Determination of the Susceptibility of Metallic Materials to Gaseous Hydrogen Embrittlement
ASTM F-1624	Standard Test Method for Measurement of Hydrogen Embrittlement Threshold in Steel by the Incremental Step Loading Technique
ASTM G-142	Standard Test Method for Determination of Susceptibility of Metals to Embrittlement in Hydrogen Containing Environments at High Pressure, High Temperature, or Both
ASTM STP-962	Hydrogen Embrittlement: Prevention and Control
CGA G-5	Hydrogen
CGA G-5.4	Standard for Piping at Consumer Locations
CGA G-5.5	Hydrogen Vent Systems
NASA Glenn Safety Manual	Chapter 6 – Hydrogen
NFPA 55	Compressed Gases and Cryogenic Fluids Code

OTHER STATES OF H_2

As mentioned in the beginning, this article focuses on the distribution of gaseous H_2. Nevertheless, it is worth taking a brief look at two other states of H_2 — liquid and slush H_2.

H_2 in its liquid state is used overwhelmingly for three things: rocket fuel, as a means to economically transport H_2, and as a means to economically store H_2 in large volumes for gaseous H_2 distribution.

Slush H_2 is H_2 that is held at what is referred to as the fluid's triple point. The triple point in thermodynamics is the point of specific pressure and temperature at which a substance can be held at its coincident gaseous, liquid and solid states. With H_2, this is achieved at 13.81K (–434.81°F) at a pressure of 7.042 kPa (1.02 psi). This coincident state of H_2 resembles a slush. Slush H_2 is currently under consideration as a replacement aerospace fuel for liquid H_2.

Because these two states of hydrogen (liquid and slush) are relegated more to transport, storage and aerospace fuel, they are beyond the subject matter of gaseous H_2 distribution and deserve their own literary space on the topics of H_2 transport, storage, and the more exotic aerospace fuel. ❒

oline vapor. This means that in an outside installation, H_2 gas will rapidly rise and disperse, mitigating any evidence there is even a leak. But this can be a double-edged sword. If welding should be done on an outside installation above or downwind in close proximity of a H_2 leak without first performing a leak detection survey prior to welding, there could be a detonation. In an enclosed facility, the H_2 gas will rise and accumulate from the ceiling down — a circumstance that allows it to build to a large volume before increasing its chances of coming into contact with an ignition source near the floor level.

Autoignition. Autoignition is the phenomenon in which a mixture of gases or vapors ignites spontaneously with no external ignition source. It is also referred to as "autogenous ignition" or "spontaneous ignition." Autoignition is dependent upon temperature, not pressure.

The *autoignition temperature* is the lowest temperature at which a fuel, in contact with air or an oxidizer, will self-heat to ignition without an external ignition source. The autoignition temperature for a monopropellant is the temperature at which it will self-heat to ignition in the absence of an oxidizer. The autoignition temperature of gaseous H_2 in air is 585°C.

The *ignition energy* is the amount of energy needed to initiate flame propagation through a combustible mixture. The minimum ignition energy is the minimum energy required for the ignition of a particular flammable mixture at a specified temperature and pressure. Minimum spark ignition energy for gaseous

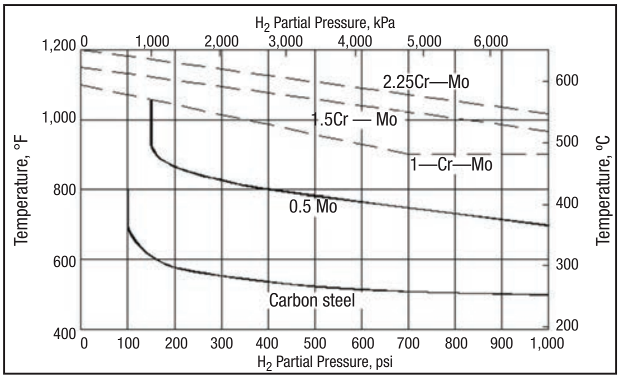


FIGURE 3. This modified Nelson diagram (adapted from API 941) can be used for selecting the right material for hydrogen service at different temperatures

H_2 in air at 1 atm = 1.9×10^{-8} Btu (0.02 mJ).

Explosive limits are the maximum and minimum concentrations of vapor, mist, or dust in air or oxygen at which explosions occur. The size and geometry of the environment as well as the concentration of the fuel control the limits. "Detonation limit" is sometimes used as a synonym for "explosive limits."

The explosive limits for a mixture of H_2 in air are 18.3 vol.% (lower limit) and 59 vol.% (upper limit).

Piping materials

In the design of piping systems (Figure 1), one of the first steps in the process will be to determine the material of construction needed for each fluid service. And each fluid service will be categorized in accordance with ASME B31.3 para. 300(b)(1), which states that, "The owner is also responsible for designating piping in Category D, Category M, High Pressure, and High Purity Fluid Services, and for determining if a specific Quality System is to be employed."

Categorizing a fluid service identifies the degree of examination and the types of examination that are required along with a number of other requirements based on a fluid's category. The owner's responsibility for this will typically fall to the owner's engineering department or an outsourced engineer.

And while the B31.3 Process Piping Code does not tell an owner what material to use for specific fluid services, it does give guidance for a material's strength, thickness and joining requirements. There are also two statements within the Introduction of the Code that are explicit in stating that:

- "It is the owner's responsibility to select the Code Section that most nearly applies to a proposed piping installation."
- "The Code is not a design handbook. Many decisions that must be made to produce a sound piping installation are not specified in detail within this Code. The Code does not serve as a substitute for sound engineering judgments by the owner and the designer."

And to expand on the first bullet point above, B31.3 Para. 300(b)(1) also states that, "The owner of a piping installation shall have overall responsibility for compliance with this Code, and for establishing the requirements for design, construction, examination, inspection and testing that will govern the entire fluid handling or process installation of which the piping is a part." Having therefore set a few ground rules for responsibilities and the requirement for designating fluid service categories, let's see where gaseous hydrogen fits into all of this.

Because of, and aside from, its tendency as a leak-prone, volatile fluid, gaseous hydrogen can be, in accordance with B31.3 fluid service categories, considered either a Normal Fluid service or a Category M fluid service. As mentioned above, categorizing a fluid service is the owner's call, so long as it fits within a selected Category guideline as described in B31.3, para. 300.2 Definitions, under "fluid service." Following are definitions of both Normal Fluid service and Category M Fluid service:

"Normal Fluid Service: a fluid service pertaining to most piping covered by this Code, i.e., not subject to the rules for Category D, Category M, Elevated Temperature, High Pressure, or High Purity Fluid Service.

Category M Fluid Service: a fluid service in which both of the following apply:

(1) the fluid is so highly toxic that a single exposure to a very small quantity of the fluid, caused by leakage, can produce serious irreversible harm to persons on breathing or bodily contact, even when prompt restorative measures are taken

(2) after consideration of piping design, experience, service conditions, and location, the owner determines that the requirements for Normal Fluid Service do not sufficiently provide the leak tightness required to protect personnel from exposure."

In the above definition for Category M, gaseous hydrogen does not meet the criteria for item (1) because it is not considered a toxic fluid. But the Code leaves the door open to enable the assignment of a fluid service as Category M by applying paragraph (2) in stating that after due consideration of "…piping design, experience, service conditions, and location…" the owner can indeed make the determination that the requirements for Normal Fluid Service do

TABLE 2. EXAMPLE SPECIFICATION FOR H_2 SERVICE

Pipe	Sch. 80, C.S., ASTM A106 Gr. B
Fittings	Sch. 80, B.W., carbon steel, ASTM A234 Gr. WPB, ASME B16.9
Flanges	R.F. Welding neck, carbon steel, ASTM A105, ASME B16.5, 300 Class
Bolts	Stud bolts, ASTM A193 Gr B7, with nuts, ASTM A194 Gr 2H
Gaskets	(Manufacturer) or equal gasket, 0.125-in. thick. 316 stainless-steel serrated solid-metal core, with spiral-wound flexible graphite both sides, and integral centering ring
Valves	
Gate	B.W. or flanged, bellows seal gate valve, welded bonnet, stainless-steel bellows, test port – (Manufacturer) #B-(size code)-2-06-4T-02-TS or equal.
Globe	B.W. or flanged, bellows seal globe valve, welded bonnet, stainless-steel bellows, test port – (Manufacturer) # B-(size code)-2-07-4T-02-TS or equal.

not sufficiently meet the needs for ensuring a heightened level of integrity in the design, construction, examination, inspection and testing of a gaseous hydrogen piping system.

Hydrogen embrittlement

Before touching on high-temperature hydrogen attack (HTHA), please refer to Table 1. In this table are a list of codes, standards, and regulations that include six documents on the topic of hydrogen embrittlement (HE), a generalized corrosion anomaly that includes HTHA. HE can occur at low temperatures and at high temperatures. Considered a form of corrosion, it can be initiated in a number of ways while also affecting a wide range of materials.

HE comes in many forms that can be characterized as hydrogen-assisted cracking (HAC), hydrogen stress cracking (HSC), stress corrosion cracking (SCC), hydrogen-assisted corrosion cracking (HACC), hydrogen blistering (HB), hydrogen induced cracking (HIC), stress oriented hydrogen-induced cracking (SOHIC), step-wise cracking (SWC), sulfide stress cracking (SSC), soft zone cracking (SZC), and high temperature hydrogen attack (HTHA).

Taken to its simplest form, hydrogen embrittlement is the mechanics of failure at the grain boundary of metals, causing a reduction of ductility as a result of the permeation of atomic hydrogen. The means by which this occurs is varied and somewhat identified by the respective titles, such as HTHA, in which the coincident high temperature and high pressure of hydrogen are the requisites for embrittlement, and SSC, in which atomic hydrogen is produced as an off-gas resulting from acid corrosion with the hydrogen then permeating the metal containment to potentially cause embrittlement. But the general result is the same with all of the above hydrogen embrittlement cases in which the strength of a metal is reduced below its allowable stress range through embrittlement, in turn setting the stage for a possible catastrophic event, given the volatility of the fluid.

With regard to material selection for gaseous H_2 service, there are two main considerations, beyond that of wall thickness and mechanical joint ratings: 1. high-temperature hydrogen attack (HTHA) and 2. the deep concern regarding leak potential. Both of these topics are now discussed.

HTHA

Atomic hydrogen, as opposed to molecular hydrogen, can propagate, among other ways, by means of hydrogen being put under elevated pressures at elevated temperatures, which sets the stage for potential HTHA. At these conditions, atomic hydrogen is able to diffuse into carbon-steel piping material or equipment, where it reacts with the carbon in solution with the metal to form methane gas at the grain boundaries. Unable to escape, the gas expands to create fissures and cracks in the pipe or vessel wall — this is HTHA. You can see clearly the results of HTHA in Figure 2, where the fissures and cracks are apparent in the wall of the 8-in. nominal pipe size (NPS) section of piping that failed under these conditions.

Carbon steel is acceptable for use in hydrogen service when operating temperatures remain below 500°F. HTHA occurs, as mentioned above, when hydrogen is contained under high partial pressure in combination with high temperatures. When the partial pressure of hydrogen is expected to be approximately 3,000 psig, at coincidental temperatures above approximately 450°F, which is what the conditions were for the Figure 2 catastrophe, then carbon steel is not recommended.

As can be seen by the modified Nelson diagram in Figure 3, as taken in part from API 941, elevated temperatures have the greatest ef-

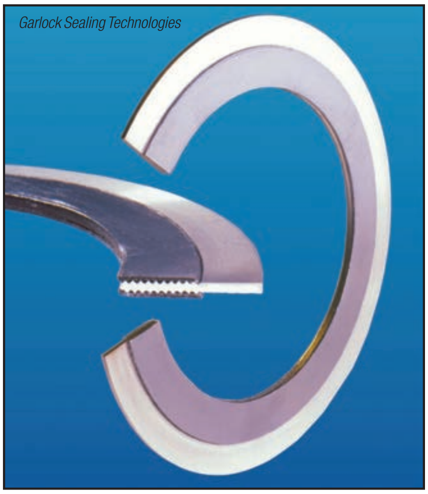


FIGURE 4. Kammprofile gaskets come with a metal core bonded with a soft filler material on both sides. After installation, the soft non-metallic filler gets pushed into the metal core serrated grooves to provide good sealing

fect in contributing to hydrogen attack. In selecting carbon steel for use in operating temperatures not exceeding 500°F, the partial pressure of hydrogen can exceed in access of 1,000 psig.

The Figure 3 diagram indicates the choice of steel warranted to avoid hydrogen attack as a function of operating temperature and partial pressure of hydrogen. Austenitic stainless steels are not susceptible to HTHA and are a satisfactory material at all temperatures and pressures.

With a proven track record, the most practical material used in hydrogen service is 316/316L austenitic stainless steel. While it is advised to post weld heat treat (PWHT) carbon steel to bake out any residual hydrogen from the welding process and decrease the post weld hardness in the heat affected zone (HAZ) this is not required for austenitic stainless steel.

Heat treatment and thermal heat effect caused by welding have little effect on the mechanical properties of austenitic stainless steel. However, the mechanical properties, such as strength and hardness of austenitic stainless steels, can be increased by cold working. When bending and forming austenitic stainless-steel pipe, its mechanical properties will be altered, including a reduction in the material's ductility.

If cold forming is required of austenitic stainless steel, a full solution anneal (heating to around 1,045°C followed by quenching or rapid cooling) will restore the material's mechanical properties to their somewhat original values. This will also remove alloy segregation, sensitization, and sigma phase realized after cold working. In performing the solution annealing process, you are cautioned that the rapid cooling might well introduce residual stresses back into the material if not done properly.

For a selection of material that is acceptable for H_2 service, Tables GR-2.1.1-1 "Material Specification Index for Piping and Pipe Components" and GR-2.1.1-2 "Material Specification Index for Pipelines" found in ASME B31.12 Hydrogen Piping and Pipelines are a good place to start.

TABLE 3. LEAK RATE ACCUMULATION

Leak rate	Unit of measure	Hours to accumulate 1ft^3	ft^3/yr
10^{-4}	cm^3/s	78,669	0.11
10^{-3}	cm^3/s	7,866.9	1.11
10^{-2}	cm^3/s	786.7	11.13
10^{-1}	cm^3/s	78.7	111.31

Mitigating leaks

With a standard atomic weight of 1.008 atomic mass units (amu), hydrogen is the lightest and smallest element in the periodic tables, giving it a high propensity to leak; with, I might add, potentially devastating results. It is therefore imperative that a gaseous piping system be designed to limit mechanical type joints and enhance those joints that are truly necessary.

In limiting potential leak points, the system should be entirely welded, with the exception of flanged joints at equipment, inline components and valving. Threaded joints should be avoided as much as possible, if not entirely. If threaded joints cannot be avoided for some reason, it is recommended that they be fully engaged without thread sealant then seal welded. Piping joints should be buttwelded, and post-weld heat treatment (PWHT) when carbon-steel pipe is used. After welding, pipe within the heat-affected zone (HAZ) becomes susceptible to hydrogen attack, even at ambient temperatures. And while hydrogen attack mainly occurs at elevated temperatures, the PWHT step will reduce, if not eliminate, that possibility entirely, even at ambient conditions.

The weak point in an all-welded system will be the flange joint. In order to provide a high degree of integrity at flanged joints, the Kammprofile gasket (Figure 4), or some form of that gasket design, should be considered. Manufactured in much the same way by multiple manufacturers, it is a very forgiving gasket. It consists of a serrated solid metal ring sandwiched between a soft, deformable sealing material. The serrations concentrate bolt load on a smaller area to provide a tight seal at lower stress. Its design allows it to compensate for irregularities in the flange surfaces as well as fluctuations in service conditions.

Another consideration in system integrity is the valving. Leaks around valve stem packing and body flanges is a real concern. In an effort to prevent this, the selection of bellows seal valves are recommended.

Using a 1-in. sch. 80 carbon steel pipe, in our following example, per ASTM A106 Gr B with allowance for manufacturing tolerance, corrosion, and mechanical allowances the maximum allowable working pressure (MAWP) can be calculated for temperatures up to 300°F in a two-step process. (Note: The reason it states, "…for temperatures up to 300ºF…" is due to the fact that the allowable stress (S) for ASTM A106 Gr B material begins to deteriorate when the temperature exceeds 300ºF. (S), in Equation (1) would therefore need to be adjusted for temperatures above 300ºF.)

Referring to Equation (1), the first step requires calculating for the theoretical burst pressure of the pipe.

$$P = (2 \times T \times S)/D \qquad \textbf{(1)}$$

Where:
D = Outside diameter of pipe, in.
P = Burst pressure, psig
P_a = Maximum Allowable Working Pressure (MAWP), psig
S = Maximum allowable stress for the material at design temperature, psi
T = Pipe wall thickness minus mechanical allowance, corrosion allowance, and manufacturing tolerance, in.

The second part of the process is to calculate for the maximum allowable working pressure, P_a, for the pipe by applying a safety factor, S_f, against the results for P in accordance with Equation (2):

$$P_a = P/S_f \qquad \textbf{(2)}$$

Therefore, in using the 1-in. sch. 80 material mentioned above, the calculation for the burst pressure would look like the following:

$P = (2 \times 0.107 \times 20{,}000)/1.315$
$= 3{,}254$ psig
= Theoretical burst pressure

By then applying a safety, S_f, of 4, as recommended in the ASME Pressure Vessel Code Section VIII-1 2019, para. UG-101, the calculation would look like the following:

$P_a = 3{,}254/4 = 813.5$ psig, or say 810 psig MAWP

The resulting 810 psig MAWP applies to the pipe only. The flange joints, or the lowest rated component in the system will be the governing factor in determining the allowable pressure for the system.

Based on ASME B16.5, at temperatures from –20°F to 100°F, the Class 150 carbon-steel flange joint has a maximum allowable working pressure of 285 psig. Class 300 has a maximum allowable working pressure of 740 psig. This will be the limiting pressure-containing factor for the system as per the following material specification example. And additionally, those values can be exceeded by a factor of 1.5 for hydrotesting only.

Example specification

As an example for a basic carbon-steel material specification, a pipe specification for gaseous H_2 service operating at ambient temperatures with design pressures below 740 psig might consist of the material requirements shown in Table 3. The following are the types of notes that might be included in the specification:

1. Examination shall include 100% radiography or ultrasonic examination of all welds.
2. Installation should minimize or eliminate the use of breakout flanges. Flange joints should only exist at flanged equipment, including instruments, and flanged valves.
3. When a carbon-steel-to-carbon steel threaded connection is required, do not apply thread compound during assembly. Seal-weld after full thread engagement.
4. Examine 100% of buttwelds by non-destructive testing (NDT) methods, such as radiography or ultrasonic, prior to PWHT. Document the examination process.
5. Welds shall be post weld heat treated. PWHT is required to prevent HTHA of the pipe weld seam and material around the heat affected zone at weld joints. The service provider shall provide documentation of the PWHT process. As an alternative, weld metal hardness controls can be put in place such that the maximum weld metal hardness in carbon steel is equal to or less than 200BHN and weld procedure qualification testing shall be done to ensure that the hardness of the heat-affected zone (HAZ) at each weld does not exceed 248 VHN (reference: NACE RP0472).
6. The maximum design limit is based on the weakest component in the system. It is not based strictly on the maximum temperature or maximum pressure of the component, but on the highest allowable coincident of the two.

Honorable mention

There are many elements, other than the pipe itself, that make up a piping system, such as fittings, valves, inline equipment, and so on. And while many of these items would be incorporated to make up a piping system to discuss them at length would require more pages than this article can accommodate.

Having said that, the same information found in this article can also be applied to the fittings, valves and inline equipment that make up a gaseous hydrogen piping system.

Leak testing

When installing a piping system for a material as potentially volatile as H_2 a procedure for leak testing should be established that not only sets forth thorough and definitive guidelines, but also identifies the best suitable means of assuring system integrity.

Part of that assurance lies with the leak testing procedure. Using a two-

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step procedure wherein the first step is a pneumatic leak test for pressure integrity followed by a sensitive leak test for leak integrity. Both tests are in accordance with ASME B31.3, ensuring the integrity of the joints with a close approximation of the H_2 service gas and its leak potential.

Aside from hydrogen's potential volatility, its molecular size, with an atomic mass of 1.008 amu, creates a containment problem. (The reason for the follow-up sensitive leak test.) Helium, with an atomic mass of 4.002602 amu, provides a very close approximation of that containment problem. Nitrogen, with an atomic mass of 14.00674 amu, would not provide the same assurances found when using helium as the test gas. I would recommend against using a heavier gas for the leak test, such as nitrogen, by then extrapolating the results of a nitrogen leak rate to determine what the leak rate might be if it were H_2.

When testing potentially volatile or lethal piping systems for leaks, a maximum allowable leak rate should be predetermined and specified. The quantitative aspect of the accumulation of H_2 from a leak can be assessed under two separate criteria:

1. Is the piping inside a building?

a. Is the building well ventilated?

b. Are there any potential ignition sources within close proximity to the piping?

c. Is the piping in an area that could pocket and accumulate hydrogen emission?

2. Is the piping in open air?

a. Are there potential ignition sources within close proximity to the piping?

Two different acceptable leak rates could be established for inside piping systems and outside piping systems. The high diffusion rate of helium makes it difficult to test for minute quantities of helium on an inside installation, and even more difficult on an outside installation. For that reason, and because H_2 would probably not have a place to accumulate outside, a higher leak rate could be tolerated for an outside installation.

Detecting leaks can be accomplished with a soapy water solution like Snoop. However, this is not the best method for locating the relatively small leaks that could occur with helium. Nor does it provide a means to quantify the leak rate.

Using a helium probe (spectrometer), leak rates can be determined to a level of 10^{-6} cm^3/s. This allows leaks to not only be located but to be quantified as well. Determining and specifying the maximum allowable leak rate for gaseous hydrogen is a plant- or owner-specific issue that is based on a plant by plant circumstance.

If it is determined that a single maximum allowable leak rate would apply to both inside and outside installations, then the basis for a worse case inside installation would determine the maximum allowable leak rate. In making that determination, a scenario would have to be created whereas a leak would occur at a joint, at an assumed leak rate, inside a building, in still air, with a vaulted or penthouse-type ceiling; a space above the leak where H_2 could accumulate.

Assuming good design practices have been followed, the main concern regarding this discussion is with a gaseous H_2 discharge from a leak accumulating in an enclosed building. Table 3 lends some perspective when assessing the magnitude of a given leak rate.

When setting a value for an allowable leak rate, it should be assumed that good design practices may not be adhered to. Even though a good design, particularly where H_2 is concerned, would not allow a building to be designed without good ventilation, and would not allow a penthouse type ceiling without ventilation, it should be assumed otherwise; a worst case scenario, if you will.

As a reference, ASME B31.3 – Process Piping provides for a Sensitive Leak Test in Para. 345.8, subparagraph 345.8.2 Method, in which it states that, "The test shall be the Bubble Test — Direct Pressure Technique in accordance with ASME BPVC, Section V, Article 10, Mandatory Appendix I or another leak test method that has a demonstrated sensitivity not less than 10^{-3} std. mL/s under test conditions."

Final remarks

Whether you're designing a low-pressure gaseous H_2 distribution system at ambient temperatures or a resid-hydrotreater system operating in the neighborhood of 3,000 psig at 600°F, engineering and construction need to go into it with a good understanding of the many risk nuances that H_2 brings to the table.

As mentioned a number of times, H_2 is very volatile and unforgiving. Do the design and construction as if you were the one who had to work around such a system every day. That kind of mindset brings a whole new perspective to what you are doing.

The list of codes, standards and a regulation in Table 1 provide a wealth of information regarding the design and construction of hydrogen piping systems. I would recommend gaining access to the information contained in these volumes prior to getting involved with designing and constructing a H_2 system. Understanding the nuances in H_2 piping design helps you avoid the pitfalls you might otherwise overlook. ■

Edited by Gerald Ondrey

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Hazardous Materials: What to Do When Disaster Strikes

Detailed plans for handling hazardous materials should be a central part of any chemical plant's disaster preparedness plan

Wade Scheel
Clean Earth

Over the past year, many chemical facilities managed to overcome extreme circumstances. One instance of an extreme event was the winter storm in Texas in February 2021, where unexpected weather conditions resulted in widespread power outages and mass water supply shortages.

Due to power-grid failures, it is estimated that the storm caused blackouts for over 5.2 million homes and businesses, becoming one of the largest blackout events in modern American history [*1*]. This highlighted the need to be prepared for all aspects of how energy impacts a business' operations. A lack of a primary energy source, as well as a water supply, could impact a facility's ability to function safely.

Though many consider disasters to encompass only "natural" geologic and meteorological processes — storms, floods, hurricanes, tornadoes, volcanic eruptions, earthquakes, tsunamis and others — future pandemics and similar events should also be considered in preparedness plans (Figure 1).

For example, at the onset of the COVID-19 pandemic, the Occupational Safety and Health Administration (OSHA; Washington, D.C., www.osha.gov) set safety standards to ensure that employers were better prepared and acting on the impacts of their employees' exposure to hazardous waste and other health risks as a result of the virus [*2*]. Most facilities were caught off guard by the virus and did not have personal protective equipment (PPE), such as masks and gloves, and adequate sanitizing products on hand.

Unfortunately, the frequency and intensity of extreme events like Winter Storm Uri in Texas and the pandemic seems to be trending upward. According to a March 2021 report from the United Nations Food and Agriculture Organization (FAO), natural disasters are occurring three times more often than 50 years ago [*3*]. Considering the magnitude of the destruction caused by disasters, professionals in the chemical process industries (CPI) should help their facilities prepare well in advance for these costly and potentially catastrophic events.

Any type of unprecedented event can put chemical plants at tremendous risk in terms of asset damage, environmental mishaps related to the loss of hazardous materials, and risk to personnel and the community — all of which can be both costly and deadly. These risks can be reduced by proper planning and disaster preparedness. Simply put — it is vital for facilities to reassess operations and worst-case scenario assumptions.

Disasters can create significant health and safety risks for the individuals who work within CPI facilities, often in the form of hazardous waste spills and leaks. Potential environmental risks also include air, water, ground or soil contamination due to runoff (Figure 2).

To reduce the risks of injury, environmental harm or regulatory penalties, a successful disaster response requires extensive expertise and knowledge of hazardous materials and waste management, including applicable procedures and regulations.

This article discusses some hazardous wastes that are common in CPI facilities. It outlines several considerations that chemical engineers, environmental engineers and environmental, health and safety (EHS) professionals should keep in mind when handling waste streams before, during and after flooding, high winds and other extreme weather conditions or unexpected events.

FIGURE 1. A chemical plant's emergency-response plan should consider not only natural disasters, such as major storms or earthquakes, but also unprecedented events, such as future pandemics

Defining hazardous-waste types

The U.S. Environmental Protection Agency (EPA; Washington, D.C.; www.epa.gov) defines hazardous waste as "waste with properties that make it dangerous or capable of having a harmful effect on human health or the environment." It is generated from many sources, ranging from industrial manufacturing process wastes to batteries and may come in many forms, including liquids, solids, gases and sludges, [*4*]. To learn more about hazardous waste regulations, please read Practicing Year-Round Waste Compliance, *Chem. Eng.*, Jan. 2021, pp. 42–44 [*5*].

The EPA regulates hazardous waste under the Resource Conservation and Recovery Act (RCRA), which was enacted in 1976 to ensure that these wastes are managed in a safe and compliant manner [*6*]. The growing amount of waste generated has made it increasingly important for waste-management personnel to develop strategies to manage it safely. RCRA established a framework for the proper management of hazardous wastes, and from this authority, EPA has established a comprehensive regulatory program to ensure that hazardous waste is managed safely from "cradle to grave" — a mindset that encompasses the management of waste from the time it is created, through transportation, treatment and stor-

age, until it is ultimately disposed of.

All waste generators must follow the framework established by RCRA. A hazardous waste generator is defined as any organization that produces a hazardous waste. Generators are regulated based on the amount of hazardous waste they create in a calendar month, not the size of their business or facility.

The EPA recognizes three categories of generators [7]:

1. Very Small Quantity Generators (VSQGs) generate 100 kg or less per month of hazardous waste or 1 kg or less per month of acutely hazardous waste.
2. Small Quantity Generators (SQGs) generate more than 100 kg but less than 1,000 kg of hazardous waste per month.
3. Large Quantity Generators (LQGs) generate 1,000 kg per month or more of hazardous waste, or more than 1 kg per month of acutely hazardous waste.

Many substances that are handled, stored and manufactured within chemical plants are regulated as hazardous waste. Therefore, engineers and other personnel must follow all requirements outlined within RCRA, as well as any other relevant federal, state or local regulations that dictate how to properly manage and dispose of hazardous waste.

Common hazardous wastes

Listed wastes are wastes that come from common manufacturing and industrial processes. They can also come from specific industries or can be discarded commercial products. A waste is determined to be a hazardous waste if it is specifically included on one of four lists — F, K, P or U — that are found in Part 261 of Title 40 of the Code of Federal Regulations (CFR) [8].

F-List. The F-List identifies wastes from common manufacturing and industrial processes as hazardous. Because the processes generating these wastes can occur in different sectors of the industry, F-List wastes are known as wastes from nonspecific sources. These wastes are divided into seven groups that depend on the type of manufacturing or industrial operation that creates them:

1. Spent solvent wastes
2. Electroplating and other metal-finishing wastes
3. Dioxin-based wastes
4. Waste from chlorinated aliphatic hydrocarbons production
5. Waste from wood-preserving activities
6. Sludge from petroleum refinery wastewater treatment
7. Multisource leachate

K-List. The K-List identifies hazardous wastes from specific sectors of the industry and manufacturing that are considered to be source-specific wastes. To qualify as a K-listed hazardous waste, an item must fit into one of the 13 categories on the list, and the waste must match one of the detailed K-List waste descriptions in the dedicated CFR section. The processes that generate K-List wastes are as follows:

1. Wood preservation
2. Organic chemicals manufacturing
3. Pesticides manufacturing
4. Petroleum refining
5. Veterinary pharmaceuticals manufacturing
6. Inorganic pigment manufacturing
7. Inorganic chemicals manufacturing
8. Explosives manufacturing
9. Iron and steel production
10. Primary aluminum production
11. Secondary lead processing
12. Ink formulation
13. Coking

P-and U-Lists. The P-and U-Lists designate hazardous waste as pure, commercial-grade formulations of certain unused chemicals that are being disposed of. For a waste to be considered a P- or U-List, it must meet the following criteria: the waste must contain one of the chemicals listed on the P- or U-List; the chemical in the waste must be unused; and the chemical in the waste must be in the form of a commercial chemical product.

The P-List identifies acute hazardous wastes from discarded commercial chemical products. The U-List identifies hazardous wastes from discarded commercial chemical products. Both the P- and U-listed chemicals refer to materials or products that can no longer be used for their intended purpose. However, the P-listed chemicals are referred to as acutely hazardous waste because they are very hazardous even in small amounts, such as cyanides.

Other hazardous wastes. Other hazardous wastes are known as characteristic wastes. These are wastes that exhibit any one or more of the following characteristic properties: ignitability, corrosivity, reactivity or toxicity.

Engineers at CPI facilities should consult the EPA's website for an inventory of listed and characteristic wastes. State regulatory requirements for waste generators may be more stringent than those of the federal RCRA program, so as previously said, it is crucial to check state-specific policies as well [9].

FIGURE 2. The disaster risks that chemical plants must consider include potential loss of containment of highly hazardous materials, leading to contamination of water, air or soil

Emergency contingency plans

Once hazardous wastes are classified, the next step is to not only keep up with day-to-day operations, proper waste segregation and year-round compliance — but also to account for extreme circumstances.

Being prepared for potential disasters can help CPI firms to mitigate some potential damage and safeguard employees, communities and the environment. Outlined here and in the following sections are several steps to take to protect facilities in the event of a disaster.

Every large CPI facility should have a contingency plan in place for extreme weather events, which includes an emergency response plan. Some third-party waste management providers may create this on a firm's behalf as part of an existing or new service agreement.

To begin, it is recommended to

FIGURE 3. A chemical plant's disaster preparedness plan should ensure that the plant has an ample stock of necessary PPE for workers, as well as other essential items

assess a facility's risk for incidents related to natural disasters. For example, a business on the Pacific coast has the greatest risk of being impacted by earthquakes, wildfires and mudslides, while a facility on the Atlantic coast may be more likely to encounter hurricanes and flooding.

A plan should be put in place before it is ever needed. That plan should consider several factors — first, engineers and plant executives should work together to determine emergency response roles. Decide who will make crucial decisions in the event of a storm and who will be involved in hazardous waste management and removal.

An ideal emergency response plan should include a proper, strategic communication protocol and chain of command. One of the biggest mistakes companies make when preparing for a natural disaster is a lack of communication. Communication that is not handled properly creates additional obstacles for organizations to overcome during and after the disaster.

Especially in the aftermath of COVID-19 and the lessons learned around the world, companies should revisit the concept of stockpiling supplies. It is important to have a certain amount of reserved supplies to manage operations through a power outage or other conditions to make sure employees can protect themselves. What can be identified now that was needed before the pandemic or the last natural disaster? This can include personal protective equipment (PPE), such as masks or gloves, sanitizing wipes, bleach, toilet paper, power generators, water reserves and more (Figure 3).

Teams should also determine how to secure all hazardous chemicals safely outside of potential flooding areas. Identify what hazardous wastes could be generated as a result of loss of containment or loss of power. Also consider what type of reporting will need to be completed after the incident.

Finally, once a plan is in place, engineers and their teams should go through exercises to work the muscles of the program. With the frequency and severity of these events increasing, it is not good enough to have a plan sitting on a shelf — teams need to go through real-life drills to understand the impact of communication and operation breakdowns. What will be done if there is not access to the items that were counted on? What if someone in the communication chain is not present during the event? What tasks are missing support that someone needs to be assigned to manage? Address these potential scenarios in the plan.

Choosing a partner

To remain compliant in the industry's ever-changing regulatory environment, it is highly recommended to work with a third-party partner that is knowledgeable in waste management. Working closely with a dedicated and experienced partner for both emergencies and day-to-day operation ensures continuity and consistent communication.

In many cases, the correct response to a disaster might not be obvious to the untrained eye because, after a disaster, hazardous wastes may look the same as non-hazardous wastes. However, hazardous wastes cannot simply be put in a trash can and taken away. Hazardous wastes need to be identified, segregated and properly disposed of to ensure compliance.

Experienced waste management experts that specialize in emergency response and planning can partner with a plant's leadership team to provide critical advisory services to help minimize risk. From the initial response to cleanup and ultimate closeout of all regulatory paperwork and reporting, this third-party partner can help to manage risk throughout the entire lifecycle.

When facing a large-scale event, emergency response organizations can assemble a nationwide network of experts, facilities, equipment and subcontractors. Managing hazardous wastes through an emergency-response specialist helps CPI plants to find proper disposal outlets and enlist expert help with onsite segregation, and also offer emergency services such as the following:

- Spill containment
- Unknown substance handling
- Cleanup services for container leaks, fuel spills and chemical spills
- Roadside cleanup of vehicle leaks
- Handling of mercury and other materials
- All-hours emergency call-center services

Emergency response providers should guarantee that their personnel have the proper safety and health certifications and experience conducting regular audits and evaluations.

Because many roads and access points may be blocked during and after a disaster, an emergency response partner should be in contact with local law enforcement organizations and emergency response teams to find out when it is safe to travel to the affected facility and begin the hazardous waste cleanup process.

Unexpected downtime following an emergency can cost the facility several hundred thousand dollars per day. The facility's goal is to reopen the impacted location as quickly and safely as possible to minimize the business interruption and get employees back to work. Without a preexisting agreement in place, it may take longer for a third-party cleanup team to access and service a location after a hurricane or natural disaster, as their priority will be to service previously contracted customers first. With that in mind, leadership teams at chemical facilities should be proactive in selecting an emergency response partner, rather than waiting until the damage has been done and a potential crisis is underway.

When it comes to managing waste streams in anticipation of a potential environmental emergency, a small amount of planning goes a long way — and so does having an understanding of the regulatory environment and how to navigate it.

Look for a partner with a national infrastructure, fleet and staff that can migrate to a region of impact, rather than selecting a regional company that might be experiencing the same extreme weather challenges. Nationwide companies also typically have access to a secondary network that is available to bring in supplies and equipment as necessary to other areas.

Additionally, facilities may often choose to contract a backup emergency response partner and require that the backup vendor have specific knowledge of the established emergency contingency plan. That vendor can then assist during extreme weather events if the primary vendor cannot respond quickly due to access issues, distance from the disposal facility, overwhelming demand for services, and other factors.

If the primary waste-management partner was not able to remove the waste from the plant and dispose of it properly in a timely manner, the damaged plant could then turn to its backup emergency response partner for contingency intervention. The backup partner is typically located in a different area than the primary one — thus, it may have access to alternative routes and disposal locations.

Partners should also be supportive in navigating the financial aspects of a crisis. During Texas' winter storm, for instance, not only were there power outages, but energy rates also spiked afterwards. To avoid this, review financial implications in contract language with the selected partner, and look for restrictions on excessive charges and fees in the event of an emergency.

Looking ahead

Despite the unforeseen circumstances of 2020, preparedness efforts have remained steady. More people in the CPI are planning for the unprecedented challenges that will inevitably take place in the future. Contingency plans are extremely important for organizations, since being unprepared can quickly cause a company to become the local or national news of the day. If a CPI company is looked upon as a leader in its arena for water, chemicals and safety, and yet there's a sudden disaster that causes a damaged water supply, there is lasting brand damage that can be done. Besides safety and compliance, this should be a motivating factor for preparedness.

Furthermore, chemical waste services, from routine waste pickups to large-scale disaster response, must be handled with the utmost professionalism and attention to detail. In addition to being expensive, any industrial waste regulatory violation or oversight — especially in the case of a natural disaster — has the potential to seriously impact employees, the public and the environment.

In the aftermath of a disaster, waste and environmental concerns are only part of a larger, more complicated picture. Every emergency situation must be managed with a commitment to safety and full compliance, and this becomes even more important when hazardous waste streams are involved. When disaster strikes, use a preparedness plan to follow all applicable regulations from beginning to end. ■

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Considerations for Solid Catalyst Loading

Special considerations must be made for loading expensive solid catalyst materials into fixed-bed and tubular reactors

John Deajon
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Most units in the chemical process industries (CPI) use complex and expensive heterogeneous catalysts aimed at improving reaction performance. Although sometimes overlooked, the solids-handling practices assocated with loading and unloading solid catalyst materials into and out of reactors can have a significant impact on the ultimate performance of the catalyst, the operation of the process and the safety of the personnel involved. Even the most highly engineered solid catalysts can exhibit reduced performance and present safety hazards if they are not correctly handled and loaded.

Efficient catalyst loading significantly increases the process unit's performance by improving the flow distribution inside the reactor and also preventing any settling of the bed, resulting in more reliable operation. This article discusses some of the potential issues that can arise from improper loading of solid catalysts and explores best practices and current technology for achieving proper loading.

Catalyst materials and usage

Catalysts, inlcuding homogeneous, heterogeneous and biological catalysts, are added to a chemical reaction to increase the reaction rate. They are manufactured globally by a number of specialized suppliers that design them to reduce environmental emissions and production costs.

FIGURE 1. Tubular reactors contain a series of tubes that contain the solid catalyst material, as shown here

Many solid hetergeneous catalyst substances have transition metals as active sites, and the desired reaction occurs on the surface of the solid. The electron structure of transition metals adsorbs reactant molecules strongly enough to allow the stabilization of a transition state for the reaction, but not so strongly as to prevent desorption of product molecules from the catalyst surface.

Cobalt is a key constituent of a number of catalyst systems used worldwide for hydrotreating and hydrodesulfurization, Fischer-Tropsch synthesis and gasoline mercaptan removal. Other catalytic applications of cobalt include production of the monomer for manufacturing polyethylene terephthalate (PET), a plastic often used for beverage containers. Precious metals, such as platinum, palladium, ruthenium and silver, are effective catalysts in many applications because of their extreme stability at high temperatures and pressures, and their inertness to chemical reactions.

The range of different ways catalysts are used is broad. In polymer production, the catalyst material is often injected into a reactor containing the monomer and hydrogen under pressure. The polymer particles are formed and removed from the reactor.

Fixed-bed reactors are the most common type of reactor for solid catalysts. These are typically cylindrical vessels filled with catalyst pellets. The gas or liquid reactants flow through the solid catalyst bed and are converted into products.

Tubular reactors/reformers consist of a series of tubes containing the catalyst (Figure 1). This type of reactor is normally used in cases where the process must be carried out at high temperatures, and where hot gases are present on the outside of the tubes. Tubular reactors are also used where the process is highly exothermic and coolant needs to be applied to the outside of the tube.

FIGURE 2. Loading of solid catalysts is often best accomplished by specialist companies with specific experience and equipment to carry out the operation

In both cases, the presence of multiple tubes makes it possible to reach and maintain the very high or low temperatures required. Achieving the temperatures needed would be difficult if a single bed was utilized.

Fluidized-bed reactors suspend small catalyst particles by the upward motion of the fluid to be reacted. The fluid is typically a gas with a flowrate high enough to mix the particles without carrying them out of the reactor. Fluidized-bed reactors are typically multiple-vessel units whereby under normal operation, the catalyst will migrate between vessels.

Catalyst handling

Catalyst handling applications involve full containment of catalysts and require very limited exposure to workers. Loading and unloading of catalyst materials is often best completed by specialist catalyst-handling companies that have the

expertise and technology to perform this work (Figure 2).

Loading and unloading encompasses a wide range of operations. Pre-bagging is basically transferring the catalyst material from its original packaging to intermediate hoppers. Screening and sieving normally involves removing the catalyst from a reactor, sieving the different-sized particles and removing the undersized solids, dust and fines from the catalyst. The screening step may be required due to a blockage at the top of the reactor, which can cause pressure-drop and flow problems. Sieving is also used to remove other materials, such as ceramic balls that can be used as an inert support in catalyst beds. In the majority of instances, the loading method is dictated by the manufacturer.

Fixed-bed reactor catalysts are usually dumped out of the reactor via a reactor catalyst dump chute, or vacuumed out from the top manway of the reactor via a catalyst vacuum truck. The materials are unloaded into drums, supersacks, flow-bins or roll-off boxes. The methods used here are generally determined by the user.

Loading methods

The following sections discuss various methods for loading solid catalyst materials.

Vacuum loading. This consists of pneumatically conveying the catalyst directly from approved packaging types into the reactor via a vacuum system. The vacuum system creates a negative vacuum on the reactor containing the catalyst material, which is then conveyed into the reactor. This method minimizes operator exposure and environmental impact, as well as eliminating the requirement for crane support.

Direct loading. The catalysts are placed in bags and the bags are lifted with cranes. They are made to pass through a dust containment system before being loaded into the reactor. There are two types of catalyst loading methods for fixed bed reactors, namely, dense loading or sock loading. Sock loading would be the least expensive loading method.

Dense loading. In dense loading, a device is used to spread the catalyst evenly in the reactor, in order to reduce void space, reduce channelling and to achieve a greater catalyst density gain. Dense loading technologies differ in their approach, with some using rotating equipment and others relying on air as a propellant to spread the catalyst. Nitrogen can be used in place of air for self-heating catalysts. Dense loading methods require constant operator attention to regulate the feed rate and avoid surges. It would normally require an operator inside the reactor to follow loading. Periodic checking of the level and evenness is required during loading.

The dense loader is set-up to load catalyst through the top manway on the reactor, if the reactor is a multi-bed reactor. The loader is set up at the inner bed tray section, loading into the lower bed.

Sock loading. Sock loading is a method in which the catalyst is transferred from a loading hopper at the top of the reactor into the catalyst bed via a flexible sleeve or sock. It typically consists of a rigid pipe attached to the discharge nozzle of the hopper at the top, and a flexible sock at the bottom. This equipment allows the catalyst-loading technician to keep the loading sock full of catalyst and prevent the catalyst from free-falling a maximum of three feet from the discharge area while loading the catalyst bed to the correct level. The sock is shortened as the loading operation continues and as the solid level increases toward the desired level of the catalyst bed. The same technique is also used to load multi-bed reactors.

Tubular reactor/reformer loading. Loading a tubular reactor requires directly filling the catalyst into each individual tube. In the past, this has been a highly labor-intensive operation, so numerous multi-tube-loading devices have been developed and are available.

Loading tubular reactors has historically presented many challenges for contractors to address. During the infancy of efforts to address the unique challenges of emptying thousands of tubes ranging in size from 0.5 to 1.5 in. in diameter, a significant portion of those efforts were focused on reductions in manpower, and reducing exposure to dust and injury, as well as lessening the physical labor the work involved.

FIGURE 3. Modern catalyst loading requires equipment like the breathing mask shown here being tested for use inside a reactor

These challenges were compounded by the need to maintain a clean, climate-controlled work environment, and the need to recover precious metals from catalysts. Also, the fines generated during catalyst-handling activities can present health hazards.

The objective of the loading operation is to consistently load fresh catalyst into the tubes while meeting the requirements for exact outages and narrow ΔP tolerances across the tube-sheet (typically 3 to 5%), without bridging the varied sizes and shapes of the catalyst particles.

In more recent years, catalyst-handling contractors have invested significantly in the development of new technologies, equipment and methods for the removal and replacement of these expensive catalysts (Figure 3).

Among the innovations resulting from the push to improve the loading of tubular reactors are multi-tube fish-tape and recovery troughs, as well as electronic differential pressure (DP) measuring devices, airlance unloading equipment and vibratory loaders. The term "fish tape" refers to catalyst guide tubes used to unload catalysts with maximum dust containment and catalyst recovery.

By employing the newer tools, reactor contractors that once used simple templates with openings matching the pitch and inner diameter of tubes observed reductions in the time required to perform catalyst changes. They also saw improvements in spent catalyst and precious metals recovery, product yields, catalyst life and the quality of the overall run cycle.

Current technology

The predominant technology employed in the U.S. tubular market

today involves loading systems that drop bulk catalyst charges from a hopper by tube volume into cartridges loaded onto ten-tube vibratory loaders. Tracking of progress and status of each tube as it is loaded is essential to avoid mistakes when so many tubes are involved.

In order to accurately track loading progress, color-coded caps cover each tube. The availability of four or five different cap colors is typically required, so if a reactor contains 10,000 tubes, up to 50,000 or 60,000 tube caps are required per reactor. The installation, removal and re-installation of these caps can be a very time-consuming, but necessary, step in the loading process. The requirement for accurate tube counts between shifts and other times is also very time consuming. For each loader inside the vessel and on the tube-sheet, a dedicated operator is required, along with a runner who delivers the filled cartridges to the loader operator.

This system also requires two or three additional personnel at the charging hopper in addition to hole watchers, ground and other support personnel. With most reactor inner diameters at 20 in. or less, the space accommodates anywhere from four to six ten-tube loaders, requiring a crew of 12 to 16 people.

Once installed, the wheeled, individual loaders are moved relatively easily via a system of tracks. These systems are electrically driven with built-in dust collection that is fairly adequate. Load results are typically good, with an average of 50 tubes at a time filled.

Next-generation loaders capable of loading 120 tubes at once, and tube-sheet cover plates that replace the need for individual tube caps, have recently become available. They include a de-dusting hopper and two stages of built-in dust collection. The pneumatically driven units have several features to prevent double loading of tubes. Tube-sheet cover plates can be custom made for each reactor, based upon reactor and tube-sheet inner diameter, tube inner diameter and pitch.

Every catalyst manufacturer will likely have recommended best practices on how to load their product into a reactor. Reputable catalyst handling companies can contribute valuble experience and special equipment to accompish the loading safely and correctly. ■

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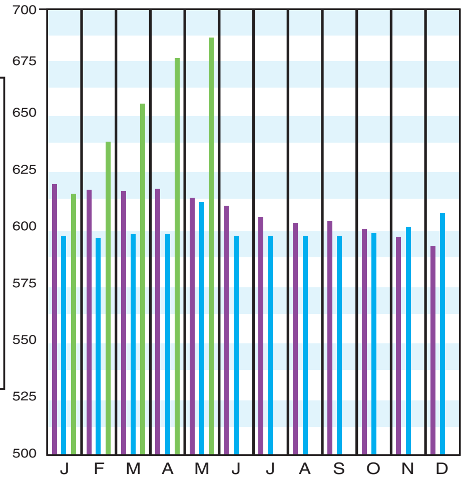
2019 2020 2021

Download the CEPCI two weeks sooner at www.chemengonline.com/pci

CHEMICAL ENGINEERING PLANT COST INDEX (CEPCI)

(1957–59 = 100)	May '21 Prelim.	Apr. '21 Final	May '20 Final
CE Index	687.3	677.1	593.5
Equipment	849.4	836.5	720.3
Heat exchangers & tanks	729.2	721.0	616.1
Process machinery	863.0	854.9	721.1
Pipe, valves & fittings	1160.6	1129.5	942.2
Process instruments	507.6	495.3	409.6
Pumps & compressors	1,115.6	1,111.4	1,086.3
Electrical equipment	601.0	593.3	561.1
Structural supports & misc.	915.0	904.5	774.0
Construction labor	341.8	340.3	333.8
Buildings	739.2	710.7	587.4
Engineering & supervision	310.4	310.3	312.6

Annual Index:
2013 = 567.3
2014 = 576.1
2015 = 556.8
2016 = 541.7
2017 = 567.5
2018 = 603.1
2019 = 607.5
2020 = 596.2

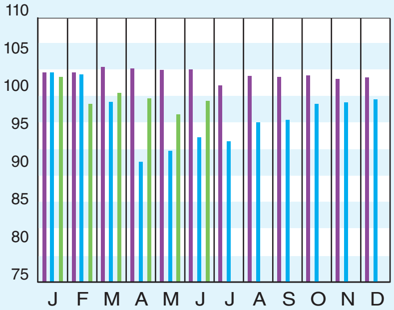


Starting in April 2007, several data series for labor and compressors were converted to accommodate series IDs discontinued by the U.S. Bureau of Labor Statistics (BLS). Starting in March 2018, the data series for chemical industry special machinery was replaced because the series was discontinued by BLS (see *Chem. Eng.*, April 2018, p. 76–77.)

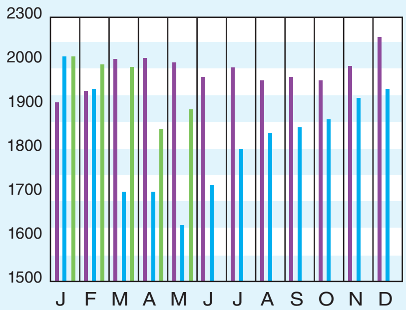
CURRENT BUSINESS INDICATORS

CURRENT BUSINESS INDICATORS	LATEST	PREVIOUS		YEAR AGO
CPI output index (2017 = 100)	Jun. '21 = 96.6	May '21 = 95.0	Apr. '21 = 95.0	Jun. '20 = 87.9
CPI value of output, $ billions	May '21 = 1,869.3	Apr. '21 = 1,761.8	Mar. '21 = 1,761.8	May '20 = 1,440.9
CPI operating rate, %	Jun. '21 = 77.0	May '21 = 75.6	Apr. '21 = 75.6	Jun. '20 = 69.6
Producer prices, industrial chemicals (1982 = 100)	Jun. '21 = 313.8	May '21 = 240.0	Apr. '21 = 240.0	Jun. '20 = 209.0
Industrial Production in Manufacturing (2017 =100)*	Jun. '21 = 97.9	May '21 = 96.8	Apr. '21 = 96.8	Jun. '20 = 89.1
Hourly earnings index, chemical & allied products (1992 = 100)	Jun. '21 = 195.1	May '21 = 194.3	Apr. '21 = 194.3	Jun. '20 = 190.6
Productivity index, chemicals & allied products (1992 = 100)	Jun. '21 = 92.1	May '21 = 92.1	Apr. '21 = 92.1	Jun. '20 = 87.8

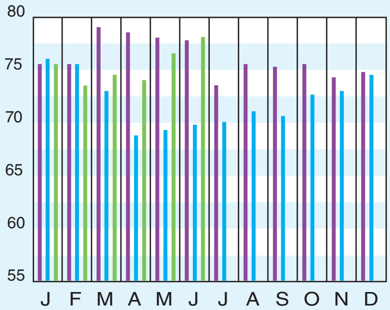
CPI OUTPUT INDEX (2007 = 100)†



CPI OUTPUT VALUE ($ BILLIONS)



CPI OPERATING RATE (%)



*Due to discontinuance, the Index of Industrial Activity has been replaced by the Industrial Production in Manufacturing index from the U.S. Federal Reserve Board.
†For the current month's CPI output index values, the base year was changed from 2012 to 2017
Current business indicators provided by Global Insight, Inc., Lexington, Mass.

CURRENT TRENDS

The preliminary value for the *CE* Plant Cost Index (CEPCI; top) for May 2021 (most recent available) is once again higher than the previous month, continuing a string of substantial monthly increases since the beginning of the year. In May, large upticks were observed in the Equipment and Buildings subindices, while the Construction Labor and Engineering & Supervision subindices saw very small rises. The current CEPCI value now sits at 15.8% higher than the corresponding value from May 2020. Meanwhile, the Current Business Indicators (middle) show increases in the CPI output index and the CPI operating rate for June 2021, and an increase in the CPI value of output for May 2021.